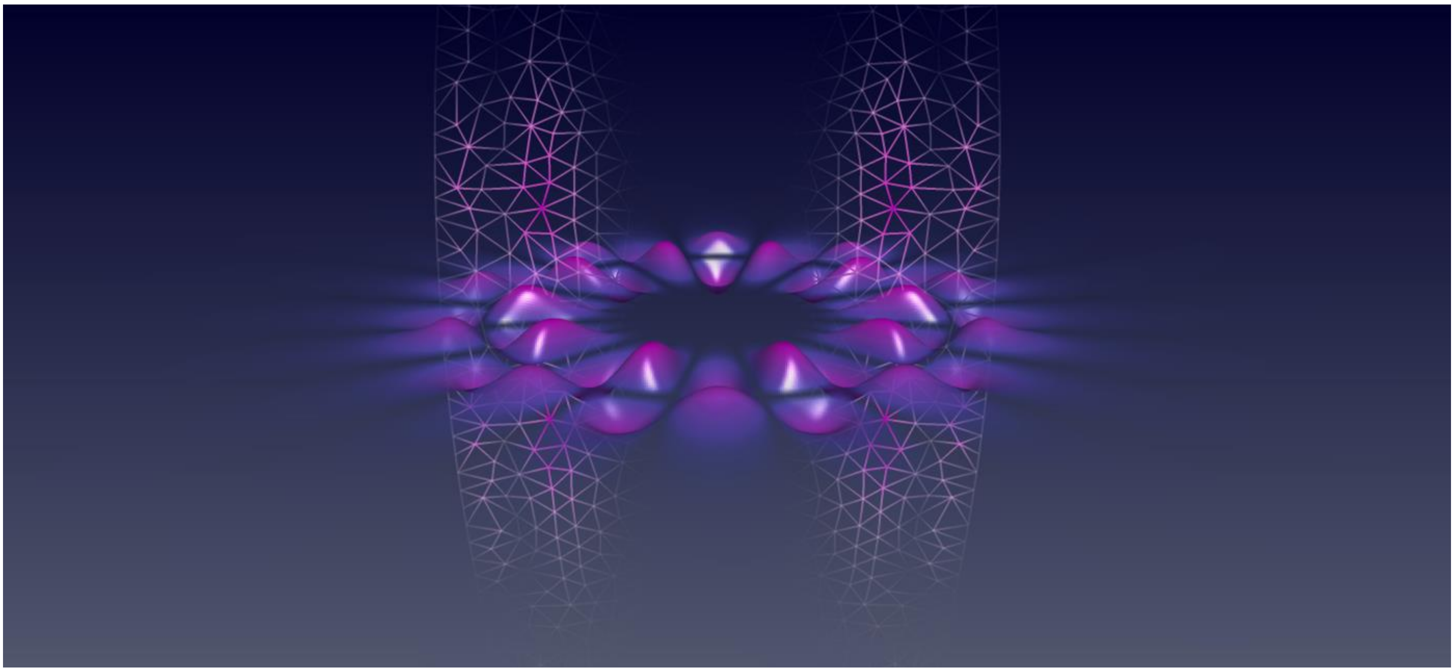
Workshop on Theoretical and Numerical Tools for Nanophotonics

TNTN 2020

comprising
OWTNM 2020 - XXVIII International Workshop on Optical Wave & Waveguide Theory and Numerical Modelling
and
13th Annual Meeting Photonic Devices



Date: 12-14 February 2020
Location: Zuse Institute Berlin, Germany

Venue

Zuse Institute Berlin
Takustraße 7
14195 Berlin
Germany

Wifi: Gast-im-ZIB

Workshop dinner:
Alter Krug Dahlem
Königin-Luise-Straße 52,
14195 Berlin

Organizers

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Wednesday

From	Speaker	Affiliation	Title
10:00	Sven Burger	Zuse Institute Berlin	Opening
10:15	Sergei Tretyakov	Aalto University	Modular analysis of arbitrary dipolar scatterers: the materiatronics concept (invited)
10:45	Rubén Esteban	Donostia International Physics Center, Donostia-San Sebastián	Focusing light to the molecular scale (invited)
11:15	Ulrich Hohenester	Karl-Franzens-Universität Graz	3D Imaging of Vibrational Surface Modes in a single MgO Nanocube
11:30	**Lunch Break**		
13:00	Giulia Tagliabue	École Polytechnique Fédérale de Lausanne	Controlling Light-Energy Conversion at the Nanoscale: A Synergistic Experimental and Theoretical Approach (invited)
13:30	Jan Olthaus	University of Münster	Optimal Photonic Crystal Cavities for Coupling Nanoemitters to Photonic Integrated Circuits
13:45	Jens Niegemann	Lumerical Inc., Vancouver	Inverse Design Methods using FDTD for Manufacturable Photonic Devices
14:00	Philipp-Immanuel Schneider	JCMwave GmbH, Berlin	A machine learning method for efficient design optimization
14:15	Mahmoud Elsawy	Inria Sophia Antipolis	Statistical learning optimization for highly efficient graded index photonic lens
14:30	**Coffee Break**		Group photo outside

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Wednesday

From	Speaker	Affiliation	Title
15:30	Javier García de Abajo	ICFO-Institut de Ciencies Fotoniques, Barcelona	Quantum Aspects of Electron-Light-Plasmon Interactions at the Atomic Scale (invited)
16:00	Uwe Morgner	Leibniz Universität Hannover	The virtual lab: Modelling femtosecond nonlinear light-matter interaction (invited)
16:30	Gerard Granet	Université Clermont Auvergne	Benchmarking numerical modal methods for modeling plasmonics structures
16:45	Matias Ruiz	Imperial College London	Slender body theory for plasmonic resonances
17:00	**Coffee Break**		
17:15	**Poster Session**		
19:00	**End of Day**		
19:30	**Workshop dinner**		Workshop dinner at 19:30 in the restaurant „Alter Krug“ in Berlin-Dahlem (everyone pays for their own drinks and food)

Wednesday Poster Session

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Nr.	Speaker	Affiliation	Title
1	Anastasiia Sorokina	Aalto University	Advantages and limitations of different modeling approaches for characterization of emission of light from III-V nanowires
2	Anne-Laure Fehrembach	Institut Fresnel, Marseille	Numerical modelling of second harmonic generation in large subwavelength-patterned highly resonant structures
3	Carol Rojas	Physikalisch-Technische Bundesanstalt, Braunschweig	Photonic Microring Resonators for Temperature Sensing – Multiphysics Modeling and Material Comparison
4	Carsten Henkel	Universität Potsdam	Light-Matter Interactions on the 10nm Scale – from Quantum Fields to Mechanical Forces
5	Cem Güney Torun	Humboldt-Universität zu Berlin	FE Simulation of a Dipole Emitter Coupled to an Inverted Diamond Nanocone
6	Dinesh Kumar Sharma	Indian Institute of Technology Kanpur	Micro-hole Collapsing Attributes in Microstructured Optical Fiber
7	Dmytro Kolenov	Delft University of Technology	Highly-sensitive laser focus positioning method with sub-micrometre accuracy using coherent Fourier scatterometry
8	Dominik Theobald	Karlsruher Institut für Technologie	Design of light scattering nanoparticles for improved photon management in light-emitting devices
9	Elena Romanova	Saratov State University	Nonlinear Interaction of Femtosecond Pulses with Glassy Chalcogenides
10	Evgeni Bezus	Samara University	Calculating Complex-Frequency Eigenmodes of Long-Period Photonic Crystal Slabs Using Aperiodic Fourier Modal Method
11	Felix Binkowski	Zuse Institute Berlin	Contour integral methods for computing nanophotonic resonances
12	Fridtjof Betz	Zuse Institute Berlin	Numerical realization of the Riesz projection expansion
13	Habib Mohamad	Université Grenoble Alpes	An aperiodic differential method associated with the FFF: a numerical tool for integrated optic waveguide modelization
14	Hannes Lüder	Technische Fakultät der Christian-Albrechts-Universität zu Kiel	Absolute refractive index dispersion determination from angle-resolved photonic crystal slab transmission spectra
15	Hukam Singh	Indian Institute of Technology Kanpur	Implications on Mode-Field Expansion in Microstructured Optical Fiber
16	Jan Krüger	Physikalisch-Technische Bundesanstalt, Braunschweig	Comparison of rigorous microscope simulations for metrological determination of bidirectional measurands
17	Jörn Bonse	Federal Institute for Materials Research and Testing, Berlin	The Role of Electromagnetic Scattering in the Formation of Laser-induced Periodic Surface Structures
18	Mandana Jalali	University of Duisburg-Essen	Improving a micro-toroid’s sensing limit through adding a thin dielectric shell
19	Massimo Rippa	Institute of Applied Sciences and Intelligent Systems “E. Caianiello”, Pozzuoli	Design of Octupolar nanopattern for Plasmonic sensing of Rotavirus
20	Stephanie Willms	Leibniz Universität Hannover	Two-Color Soliton Compounds
21	Sugeet Sunder	Indian Institute of Technology Delhi	Orbital Angular Momen Momentum (OAM) Modes using Photonic Lanterns
22	Sugeet Sunder	Indian Institute of Technology Delhi	Exploring the Absorption Mechanism in Numerical Boundary Conditions towards their Optimization
23	Tim Käseberg	Physikalisch-Technische Bundesanstalt, Braunschweig	Finite Element Simulation and Optimization of Inverted Plasmonic Lenses

Thursday

From	Speaker	Affiliation	Title
09:15	Rémi Carminati	Institut Langevin, Paris	Cross density of states and mode connectivity in nanophotonics (invited)
09:45	Gilles Renversez	Institut Fresnel, Marseille	Models for wave propagation in enhanced Kerr nonlinear dielectric media: applications to the spatial control of bulk nonlinearity
10:00	Kwang Jun Ahn	Ajou University	Nonlinear THz wave Transmission Control of Graphene
10:15	**Coffee Break**		
10:45	Arno Rauschen-beutel	Humboldt Universität zu Berlin	Nonreciprocal Quantum Optical Devices Based on Chiral Interaction of Confined Light with Spin-Polarized Atoms (invited)
11:15	Igor Bondarev	North Carolina Central University	Epsilon-near-zero Modes of Transdimensional Planar Metallic Nanostructures
11:30	Roman S. Savelev	ITMO University, Saint Petersburg	Engineering asymmetric coupling in two-mode nanostructured dielectric waveguides
11:45	Julius Kullig	Otto-von-Guericke-Universität Magdeburg	Microstar cavities for light confinement without reflection
12:00	**Lunch Break**		
13:30	Kevin Vynck	Laboratoire Photonique, Numérique et Nanosciences, Bordeaux	Efficient numerical methods for the analysis and design of complex nanoresonators and disordered nanostructures (invited)
14:00	Lena Ebers	Paderborn University	Lossless optical microstrip filters for semi-guided waves at oblique incidence

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Thursday

From	Speaker	Affiliation	Title
14:15	Rémi Colom	Zuse Institute Berlin	Light-management in nanotextured perovskite solar cells
14:30	Rowan W. MacQueen	Helmholtz-Zentrum Berlin	Triplet fusion photon upconversion materials: a playground at the intersection of photonics and photochemistry
14:45	Tobias Kramer	Zuse Institute Berlin	Imaging chiral structures: Polarization dependent time- and frequency resolved spectra of photosynthetic complexes
15:00	**Coffee Break**		Tour to the HLRN Supercomputer at Zuse Institute Berlin
16:00	Tobias Heindel	Technische Universität Berlin	Engineered Solid-State Quantum-Light Sources for Quantum Communication (invited)
16:30	Thorsten Feichtner	University of Würzburg	An ambient condition nanoscale electrochemic device with direct optical antenna feedback
16:45	Emilie Sakat	Laboratoire Charles Fabry, Université Paris-Saclay, Palaiseau	Upper bound of a nanovolume absorption cross-section situated in the vicinity of a nanoantenna
17:00	André Nicolet	Institut Fresnel, Marseille	Dispersive Quasi Normal Modes (DQNM) in Electrodynamics: Numerical Computation and Modal Expansion
17:15	Guillaume Demésy	Institut Fresnel, Marseille	A collection of 3D full-vector finite element models for waveguide-based plasmonic sensors
17:30	**Poster Session**		Snacks and drinks at Zuse Institute Berlin
19:30	**End of Day**		

Thursday Poster Session

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Nr.	Speaker	Affiliation	Title
1	Anne Talneau	Centre de Nanosciences et de Nanotechnologies, Palaiseau	Sub-wavelength Metamaterial for a Variable and finely Tailored Coupling Coefficient within Waveguides Arrays
2	Anna Andrle	Physikalisch-Technische Bundesanstalt, Berlin	Grazing incidence X-ray fluorescence measurement on nanostructures for element sensitive reconstruction
3	Daniel Reiche	Max-Born-Institut, Berlin	Modeling Landau Damping in Atom-Surface Quantum Friction
4	Danil Kornovan	ITMO University, Saint Petersburg	Reduction of multipole moments in subwavelength periodic dipolar chains
5	Carlo Gigli	Laboratoire Matériaux et Phénomènes Quantiques, Paris	Quasinormal mode expansion for nonlinear optical generation in subwavelength resonators
6	Fabian Loth	Humboldt-Universität zu Berlin	Surface roughness in finite element meshes
7	Gerardo Silva-Oelker	Universidad Tecnológica Metropolitana, Chile	The Shape Derivative for Uncertainty Quantification and Optimization of Perfectly Electric Conducting Gratings
8	Hamid Keshmiri	Federal Institute for Materials Research and Testing, Germany	Multi-resonant plasmonic supercells
9	Johannes Sutter	Helmholtz-Zentrum Berlin	Shallow Nano-Textures for Light Management in Solution-Processed
10	Jörg Bischoff	Technische Universität Ilmenau	Model Based Scanning Coherent Fourier Transformation Scatterometry (SCFT) – a new approach for subresolution of non-periodic nano-patterns
11	Katja Höflich	Helmholtz-Zentrum Berlin	Resonant behavior of a single plasmonic helix
12	Lucas Rickert	Technische Universität Berlin	Optimized designs for telecom-wavelength quantum light sources based on hybrid circular Bragg gratings
13	Manfred Hammer	Paderborn University	Small-scale online simulations in guided-wave photonics
14	Marian Marciniak	National Institute of Tele-communications, Warsaw	From Nano-Optics to Quantum Mechanics: Method of Single Expression Extends its Domains
15	Meiping Yu	Laboratoire Charles Fabry, Université Paris-Saclay, Palaiseau	Quasinormal Modes Expansion Techniques: Study of the Convergence Rate
16	Mohamed Ghobara	Freie Universität Berlin	Diatom frustules: A biomaterial with promising photonic properties
17	Samer Alhaddad	Paderborn University	HighPerMeshes as a framework for numerical simulations
18	Tobias Grunewald	Physikalisch-Technische Bundesanstalt, Braunschweig	Analysis of ellipsometric layer thickness measurements employing a new merit function for depolarizing Mueller matrices
19	Tong Wu	Laboratoire Photonique, Numérique et Nanosciences, Bordeaux	Multipolar decomposition of quasi-normal modes: a new design tool for nano-optics
20	Ugur Meric Gur	Technical University of Denmark	Analysis of Open Elliptical Nanophotonic Structures with the Modal Method
21	Vadim Razukov	Yuri Gagarin State Technical University of Saratov	Ultra-short Optical Pulse Dynamics in Bidirectional Ring Fibre Cavity
22	Yuri Rapoport	Taras Shevchenko National University of Kyiv	New Physical Phenomena: Switching of Focusing and Chaotic Field Behavior in Strongly Nonlinear Active Hyperbolic Concentrator
23	Yuri Rapoport	Taras Shevchenko National University of Kyiv	Wave Processes in Tunable Layered, Nonlinear, Active and Mesoscale Hyperbolic and Dielectric-Graphene Metamaterials
24	Xavier Garcia Santiago	Karlsruher Institut für Technologie	Global optimization of a free-form waveguide coupler

Friday

From	Speaker	Affiliation	Title
09:00	Evgeni Bezus	Samara University	Coupled-wave analysis of bound states in the continuum in integrated nanophotonic elements for semi-guided waves (invited)
09:30	Laura Fabris	Rutgers University, New Jersey	A Holistic Computational-Experimental Approach toward Tridimensional Gold Nanostar Antennas (invited)
10:00	Christoph Pflaum	Friedrich-Alexander Universität Erlangen-Nürnberg	Beam Propagation Methods for Laser Amplifier Simulation
10:15	**Coffee Break**		
11:00	Martijn Wubs	Technical University of Denmark, Lyngby	Quantum Plasmons in Graphene Nanoribbons: New Insights from Continuum and Atomistic Theories (invited)
11:30	Yannick Augenstein	Karlsruher Institut für Technologie	Material reparametrization for topology optimization of 3D photonic nanostructures
11:45	Bernard Kapidani	Technische Universität Wien	A high-order accurate, explicit in time, extension of the FDTD/FIT algorithm to triangular meshes
12:00	Paul Mertin	University of Kassel	Numerical Analysis of Emitter Coupling in Photonic Crystal Cavities using Green’s Function
12:15	Frank Schmidt	Zuse Institute Berlin	Causality as Construction Principle for Transparent Boundary Conditions
12:30	**Lunch Break**		
14:00	Francesco Intravaia	Humboldt Universität zu Berlin	Investigating electromagnetic fluctuation-induced interactions (invited)

Friday

From	Speaker	Affiliation	Title
14:30	Dan-Nha Huynh	Humboldt-Universität zu Berlin	Different Approaches to the Hydrodynamic Material Model within the Discontinuous Galerkin Time-Domain Method
14:45	Doguscan Ahiboz	Helmholtz-Zentrum Berlin	Adjustable Dielectric Metasurface for Enhanced Photon Up-Conversion
15:00	Phillip Manley	Helmholtz-Zentrum Berlin	Simulation of Metasurface Enhanced Photon Up-Conversion
15:15	**End of Day**		Closing remarks

Supported by

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Book of abstracts

Invited talks

Nonreciprocal Quantum Optical Devices Based on Chiral Interaction of Confined Light with Spin-Polarized Atoms

Arno Rauschenbeutel [1]

[1] *Department of Physics, Humboldt-Universität zu Berlin, Germany*

Tightly confined light fields exhibit an inherent link between local polarization and propagation direction. Their interaction with quantum emitters therefore features propagation-direction-dependent effects which are interesting both conceptually and for applications in quantum photonics.

The confinement of light in nanophotonic structures results in an inherent link between the light's local polarization and its propagation direction [1]. Remarkably, this leads to chiral, i.e., propagation-direction-dependent effects in the emission and absorption of light by quantum emitters [2]. We employed this effect to demonstrate an integrated optical isolator [3] as well as an integrated optical circulator [4] which operate at the single-photon level and which exhibit low loss. These are the first two examples of a new class of nonreciprocal nanophotonic devices which exploit the chiral interaction of quantum emitters with transversally confined photons.

References

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Coupled-Wave Analysis of Bound States in the Continuum in Integrated Nanophotonic Elements for Semi-Guided Waves

E. A. Bezus [1,2], D. A. Bykov [1,2], L. L. Doskolovich [1,2],

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[2] *Samara National Research University, 34 Moskovskoye shosse, Samara 443086, Russia*

We theoretically and numerically study bound states in the continuum (BICs) supported by integrated nanophotonic elements for semi-guided waves, which consist of one or several dielectric ridges located on the surface of a dielectric slab waveguide or terminating it. We derive simple but extremely accurate coupled-wave models that prove the BIC existence and enable predicting their positions in the parameter space. The developed models show that the investigated BICs are topologically protected and, hence, robust to small changes in the parameters of the nanophotonic element.

Bound states in the continuum in integrated nanophotonic elements

Bound states in the continuum in photonics are non-leaky eigenmodes, which are supported by resonant photonic structures having open scattering channels [1]. In recent years, investigation of BICs has attracted considerable attention not only due to the fundamental interest, but also due to many potential applications in lasing, filtering and sensing, among others.

In the present work, we study the formation of high-Q resonances and BICs in simple integrated nanophotonic elements for semi-guided waves (plane-wave-like modes of a dielectric slab waveguide [2]) consisting of dielectric ridges located on the surface of a slab waveguide [3] or terminating it [4]. Using rigorous numerical simulations based on the aperiodic Fourier modal method, we show that such ridges support robust BICs. We investigate the interaction of the BICs governed by their topological properties and demonstrate that they can coalesce and annihilate, leading to the so-called strong resonance effect [4]. The existence of high-Q resonances and BICs in the investigated nanophotonic elements makes them promising for designing spectral and spatial integrated filters for semi-guided waves [5]. The derived coupled-wave models describing bound states in the continuum can be applied to other photonic structures, e.g. guided-mode resonant gratings [6].

Acknowledgments

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Investigating electromagnetic fluctuation-induced interactions

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Electromagnetic fluctuation-induced interactions play an important role in many area of science and their investigation is becoming essential for nano- and quantum-technologies. We will review the physics behind these phenomena, highlighting with some recent results the relevance of the system's geometry and optical properties.

The importance of fluctuations in physics is often underestimated and they are usually seen as a nuisance which should be eliminated. However, fluctuations induce and/or dominate a large number of phenomena which are relevant to many areas of science. Prominent examples of these phenomena are dispersion forces, like the van der Waals and the Casimir interaction. They play an important role in the functioning micro- or nanoelectromechanical systems [2, 3], in atom-chip technologies [4] and in fundamental research, ranging from material sciences (e.g. van der Waals materials) [5] to the search for modifications of the law of gravity [6].

The study of fluctuation-induced phenomena is highly multidisciplinary and often requires an all-around perspective on how different topics of physics merge in the microscopic and mesoscopic world. Particularly important is the role played by the system's geometry and the materials' optical response. Previous work showed indeed that the interaction strength and even its sign can be strongly modified by leveraging on these properties [7, 8, 9, 10].

Modern experiments have also created new challenges for theoreticians. Commonly used approximations in the framework of quantum-optics [11] or nonequilibrium physics [12] can be inadequate for fluctuation-induced interactions. Interesting and unexpected behaviors can appear [13, 14, 15, 16]. Not the least, as soon as non-trivial geometries are involved, analytic investigations of these phenomena become prohibitive and flexible numerical schemes, allowing for a broad class of material models, have to be developed.

Here, we review some recent results on electromagnetic fluctuation-induced interactions illustrating the physics behind these phenomena and some of the approaches that have been used for their analysis.

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Controlling Light-Energy Conversion at the Nanoscale: A Synergistic Experimental and Theoretical Approach

Giulia Tagliabue

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Nanophotonic design has opened new opportunities for manipulating light energy conversion into charge carriers or heat at the nanoscale. Here we present a synergistic experimental and theoretical study of plasmonic hot-hole devices.

Light-energy conversion devices typically exploit the generation of charge carriers or heat to produce macroscopic currents and temperature gradients. By dramatically reducing the size of the light-absorbing elements to dimensions comparable to the characteristic mean-free paths of electrons and phonons, nanophotonic design has opened new opportunities for controlling and manipulating the process of light-energy conversion. In particular, highly-absorbing, plasmonic-metal nanostructures offer a promising route to bandgap-less ultra-fast photodetectors and broadband solar photocatalysts, due to their tunable absorption characteristics and ability to generate hot carriers[1-3]. For this reason, fundamental knowledge of hot-carrier energy distributions as well as their dynamics and associated lifetimes are necessary to adequately harness these energetic, non-equilibrium carriers. To date, experimental studies of hot carrier devices have focused almost entirely on the exploitation of hot electrons to produce a photocurrent or initiate a chemical reaction. Furthermore, numerous efforts have been devoted to understanding the temporal evolution of hot electrons within photo-excited metal nanostructures and various metal-semiconductor assemblies[4-6]. In contrast, there have been very few realizations of hot-hole based plasmonic devices and the dynamics of hot holes in metal nanostructures have remained largely unknown, despite the favorable energetics of hot holes predicted by ab-initio calculations [7].

In this talk we will show how the synergistc combination of experiments and theory is critical to correctly unravel the fundamental mechanisms occurring in non-equilibrium devices. Indeed, while measurement of these devices give access to integral quantities, theory provides the otherwise missing microscopic picture. In particular, here we report the construction, optoelectronic and photoelectrochemical characterization of plasmon-driven photodiodes and photocathodes based on a metal/p-type gallium nitride (p-GaN) heterostructure that operate within the visible regime via hot-hole injection. First, we report a photoelectrochemical platform for improving the selectivity of solar-to-fuel energy conversion via plasmonic hot-carriers [8]. Next, through solid-state measurements we elucidate the fundamental role played by the metal band structure in determining device performance [9]. Lastly, we use ultrafast transient absorption spectroscopy to show that plasmon-induced hot-hole injection from gold (Au) nanoparticles into the valence band of p-GaN occurs on a similar timescale as previous observations of hot-electron injection. Furthermore, we show that the thermalization process of hot-electrons is significantly affected by hot-hole collection by the p-GaN support [10]. Taken together, our studies substantially advance the understanding of hot-hole transfer in metal-semiconductor heterostructures and demonstrate new opportunities for expanding the scope of hot-carrier optoelectronics beyond hot-electron-based devices.

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Quantum Aspects of Electron-Light-Plasmon Interactions at the Atomic Scale

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We will discuss the simulation of several quantum aspects associated with plasmons in atomic-scale materials, including ultrafast radiative heat transfer, nonlinear optical response down to the single-photon level, quantum optics through coupling with quantum emitters, and the interaction with ultrafast electron beams.

Plasmons in atomic-scale structures exhibit intrinsic quantum phenomena related to both the finite spatial confinement and the small number of electrons on which they are supported. Their interaction with two-level emitters is also evidencing strong quantum effects. In this talk we will discuss several salient features of plasmons in atomic-scale materials, such as graphene and atomic layers of noble metals, including their ability to mediate ultrafast heat transfer [1], the generation of high harmonics [2] , their interaction with molecules and quantum emitters [3], and their extreme nonlinearity down to the single-photon level [2]. We will further discuss several intriguing characteristics of the plasmonic response of atomically thin silver crystalline films, the plasmons of which have been recently revealed experimentally [4]. We will conclude with a succinct description of quantum aspects emerging from the ultrafast plasmon-mediated interaction between femtosecond light and electron pulses [5].

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Efficient numerical methods for the analysis and design of complex nanoresonators and disordered nanostructures

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We show how quasinormal modes can help to design individual complex nanoresonators with targeted scattering properties, and introduce a new numerical method, named "Global Polarizability Matrix (GPM) method", that enables efficient modelling of large ensembles of complex nanoresonators in optical stacks.

Abstract

Controlling the interaction of light with nanoresonators is one of the spearheads of research in modern optics and photonics. Important efforts are dedicated to the design of individual nanoresonators (Mie resonators, plasmonic nanoantennas) to scatter light with tailored directionality, phase and polarization. The design is generally made by analyzing the multipolar response of the nanoresonator upon various excitations (incident angles, polarization and frequencies). Besides being computationally heavy, this strategy hardly brings physical insight into the problem at hand and often leads to designs that are not tolerant to spectral and angular variations of the excitation. The designed nanoresonators are then often placed in planar geometries, creating the so-called metasurfaces. The interaction of resonators with a stratified medium and between themselves can further enrich their optical properties, leading for instance to spectrally-selective angle-independent absorption or to controlled coupling between free-space modes and guided modes. These metasurfaces can sometimes be made by bottom-up approaches, relying on colloidal chemistry and self-assembly techniques. Theoretically predicting the optical properties of complex, disordered metasurfaces has however remained elusive up to now due to the difficulty to consider simultaneously the coherent phenomena occurring at the level of the individual nanoparticle (nano-scale) and at the level of the nanoparticle ensemble (meso-scale).

In this talk, we will discuss numerical methods to address the modelling challenges for the design and analysis of disordered nanostructures with targeted optical properties. First, we present a numerical method, based on the quasinormal mode formalism [1], to analyze and design the multipolar behavior of individual nanoresonators [2]. We show how the complex frequency and the "intrinsic multipolar content" of individual resonances can be tuned to reach designs that are tolerant to variations in frequency and incident angles. Second, we introduce a numerical method, named "Global Polarizability Matrix (GPM) method", that enables computationally efficient modelling of large ensembles of complex (non-spherical) resonators in stratified media even in cases of strong near-field interactions [3].

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A Holistic Experimental-Computational Approach toward Tridimensional Gold Nanostar Antennas

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Herein we show how a holistic computational-experimental approach can be implemented toward the prediction and realization of colloidally synthesized, highly monodispersed, tridimensional gold nanostar antennas that can be tailored to address various applications, including the amplification of photogenerated current in Mo dichalcogenides.

Near field techniques, such as surface enhanced Raman spectroscopy (SERS), rely on the ability of plasmonic nanoparticles to induce localized electromagnetic field enhancements in close proximity to the metallic surface. The possibility of achieving SERS signal enhancements high enough to enable sensitive identification of analytes down to the single molecule level depends on the presence of the so-called “hot spots”, which can be located at the vertices, edges, or crevices in isolated nanoparticles or at narrow junctions between assembled nanoparticles. In turn, the presence of finely tunable hot spots correlates to the possibility of applying SERS as a reliable spectroscopic technique in the analytical and biomedical fields. Our group has worked for several years on the implementation of SERS sensing substrates and imaging tags, in which gold nanostars have demonstrated to be excellent substrates. We have also shown that when these nanostructures are conformally coated with semiconductors such as TiO_2 they can efficiently photocatalyze the evolution of hydrogen from water via near IR induced generation of hot electrons. However, for the realization of more quantitative approaches, and for a more reliable E-field manipulation, improved plasmonic platforms are necessary. For this reason, we have established a combined experimental and computational approach that has led us to synthesize by design highly monodispersed gold nanostars with localized surface plasmon resonances tunable between 600 and 2000 nm. We have measured their plasmonic response both at the single particle level (via EELS) and in ensemble averaged samples (UV-Vis and FT-IR spectroscopies), with excellent agreement with the theoretical predictions obtained with 3D finite element simulations [1]. Our calculations have also shown that these nanostars can efficiently increase photocurrent generation in MoS_2 and $MoTe_2$, if morphology (and therefore plasmonic response) and relative orientation with the dichalcogenide substrate are properly tuned [2].

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Quantum Plasmons in Graphene Nanoribbons: New Insights from Continuum and Atomistic Theories

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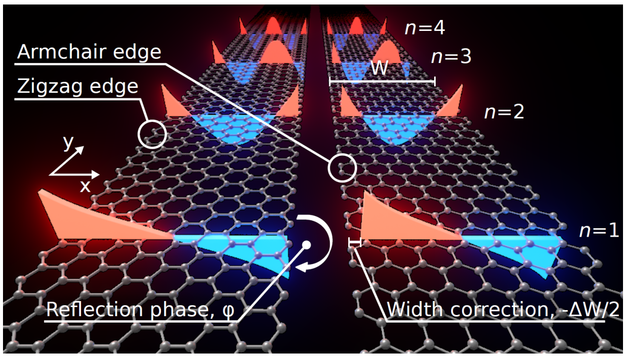
We identify a scale invariance in the Dirac theory for graphene nanoribbons. This and other insights from Dirac theory are compared to both tight-binding and density-functional calculations. We discuss the onset of nonclassical behavior, the validity of the Dirac approximation and of a Fabry-Pérot model.

Quantum plasmons on graphene nanoribbons and insight from the Dirac model

For wider graphene ribbons one can use the bulk conductivity to understand their plasmonic behavior, but quantum effects emerge for widths of the order of 10 nm. One can then use Dirac theory [1] or the more generally valid tight-binding theory [3] to understand the new properties. We find that Dirac theory can shed new light on the onset of quantum plasmonic effects in nanoribbons, and we also discuss in what part of parameter space Dirac theory for ribbons is valid [5].

We next study higher-order plasmons and whether a simple Fabry-Pérot or standing-plasmon model can be distilled from our tight-binding calculations for nanoribbons [6]. We compare our results for the reflection phase at zig-zag and arm-chair edges with previous work using continuum descriptions, for example Ref. [4].

Finally, although a continuum theory, Dirac theory predicts an interesting fine structure or sub-nanometer wave-function oscillations [2]. We show that these oscillations are well reproduced by TB and DFT calculations. Moreover, we find that this electronic fine structure carries over to a fine structure of the graphene plasmons [6].



Induced charges for dipolar and higher-order plasmons on zig-zag and armchair graphene nanoribbons. Red and blue correspond to negative and positive charges. Figure from Ref. [6].

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Cross density of states and mode connectivity in nanophotonics

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We discuss the concept of cross density of states, and its use in nanophotonics to probe the spatial extent of eigenmodes "from the inside", or to control the spontaneous emission dynamics of two classical or quantum sources in a structured environment.

We discuss the concept of cross density of states (CDOS), as a measure of the number of eigenmodes connecting two points in a structured environment [1, 2]. The CDOS, in addition to the local density of states (LDOS), drives the spontaneous emission dynamics of two classical or quantum sources in a structured environment [3, 4]. In particular, we will show that design rules can be derived for the control of the degree of quantum coherence of the light emitted by two single-photon sources [4]. From these rules, conditions for the observation of subradiant and superradiant states can be easily deduced. Based on the CDOS, we also introduce the mode connectivity, that takes the value one when the two observation points are connected by a single mode, and vanishes in the absence of modes connecting them [5]. CDOS and connectivity are useful to measure the spatial extent of eigenmodes in a complex medium. As an example, we will show that the connectivity could be used to probe Anderson localized modes in a disordered strongly scattering medium [5].

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Focusing light to the molecular scale

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We show that plasmonic resonances supported by metallic particles allow localizing light into hot-spots of subnanometer dimensions, and discuss the consequences of this confinement for molecular spectroscopy and near-field optical microscopy with (sub)molecular resolution

A main advantage of plasmonic resonances induced by the collective oscillations of the free electrons of metallic particles is their capability to localize light to dimensions much below the wavelength of the incoming light. This strong confinement of the optical fields can be exploited, for example, to improve resolution in near-field microscopy and to increase the received signal in surfaced enhanced molecular spectroscopies.

In this work, we combine classical and quantum methodologies to demonstrate the possibility to generate regions of very strong optical fields, often called hot-spots, of (sub)nanometer dimensions, and investigate the consequences for experiments. We show that these extreme hot-spots can appear for systems that combine the large plasmonic enhancement induced at the gaps between metallic structures separated by ~1 nanometer distance[1], together with a lighting-rod effect that concentrate the fields at atomically sharp features[2]. We then discuss the importance of this plasmonic-field localization for current spectroscopy measurements that have demonstrated the capability to interrogate the optical properties of molecules with sub-molecular resolution (Figure 1) [3-5] and to characterize molecular transitions that are typically dark[6-8].

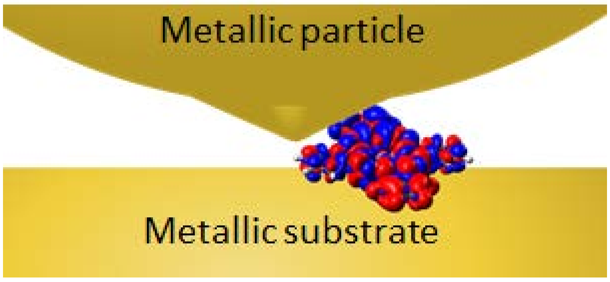

Figure 1. Example of the system under study. A plasmonic structure focuses light to a hot-spot of atomic-scale dimensions, which is exploited to characterize a molecule with (sub)nanometer resolution.

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Modular analysis of arbitrary dipolar scatterers: the materiatronics concept

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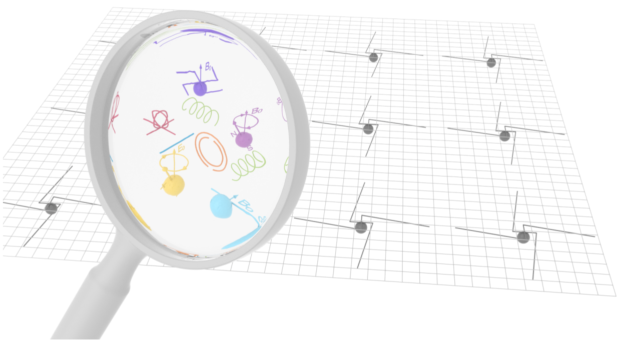
Within the paradigm of metamaterials and metasurfaces, electromagnetic properties of composite materials can be engineered by shaping and tuning their constituents, so-called meta-atoms. Synthesis and analysis of complex-shape meta-atoms with general polarization properties is a challenging task. In this presentation we will discuss our recent results on conceptual decomposion of general polarization phenomena into a set of basic, fundamental effects, which enables immediate all-direction characterization of electromagnetic properties of arbitrary linear materials and metamaterials. This platform of modular characterization (which we call "materiatronics") is tested on several examples of bianisotropic and nonreciprocal meta-atoms. The analytical approach is supported by a ready-to-use computational code and can be further extended to meta-atoms engineered for other types of wave interactions, such as acoustics and mechanics.

Theory

The decomposition principle is illustrated in the picture below. This platform of transition from complex material units to basic elements ("materiatronics") is in a sense analogous to electronics, where an arbitrarily complex linear circuit is represented as a network of basic elements: capacitors, inductors, resistors, and gyrators. In electronics, when a complex circuit is represented as a combination of lumped elements, it becomes apparent what kind of elements and of what strength must be added or removed to improve or optimize the desired response. Likewise, our proposed modular analysis can also serve as a powerful tool for *understanding*, *synthesis*, and *optimization* of meta-atoms with required polarization properties. For any small (dipolar) reciprocal meta-atom the most general electromagnetic response can be viewed as a combination of electric, magnetic, chiral, and uniaxial omega coupling effects. In the presentation, we will show examples of decompositions and the use of the results for both reciprocal and nonreciprocal meat-atoms. More details can be found in paper [1].



Conceptual illustration of the modular analysis. An arbitrary scatterer (located in a two-dimensional array of equivalent scatterers in this example) with a complex polarization response is decomposed into a combination of responses from several basic modules with known basic electromagnetic properties.

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Engineered Solid-State Quantum-Light Sources for Quantum Communication

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Tremendous progress has been achieved in the engineering of solid-state-based non-classical light sources. In this context, deterministically fabricated quantum-light sources based on semiconductor quantum dots (QDs) appear to be particularly appealing [1]. Allowing for the generation of close-to-ideal flying qubits these devices are predestinated for implementations of quantum communication scenarios.

In this talk I will review our progress in this field, striving towards the ultimate goal of a global secure communication. After briefly revisiting proof-of-concept quantum key distribution (QKD) experiments, we discuss the development of state-of-the-art components for QKD, such as plug-and-play SPSs and receiver modules. In this context, we address the direct, robust, and efficient coupling of quantum light sources to optical fibers and their integration into compact Stirling cryocoolers, representing crucial steps towards applications. For this purpose, optimized device designs for operation at telecom-wavelength are evaluated via simulations based on the finite element method [2] (see Fig. 1(a)). Furthermore I report on how to optimize the performance of quantum communication scenarios implemented with QD-based SPSs. To this end we exploit two-dimensional temporal filtering and real-time security monitoring of single-photon pulses using a receiver module designed for polarization-encoded QKD (see Fig. 1(b)). The routines developed enable us to choose optimal filter settings depending on the losses of the quantum channel [3].

The findings reported are relevant for the development of QKD-secured communication networks based on quantum light sources (cf. group website [4]).

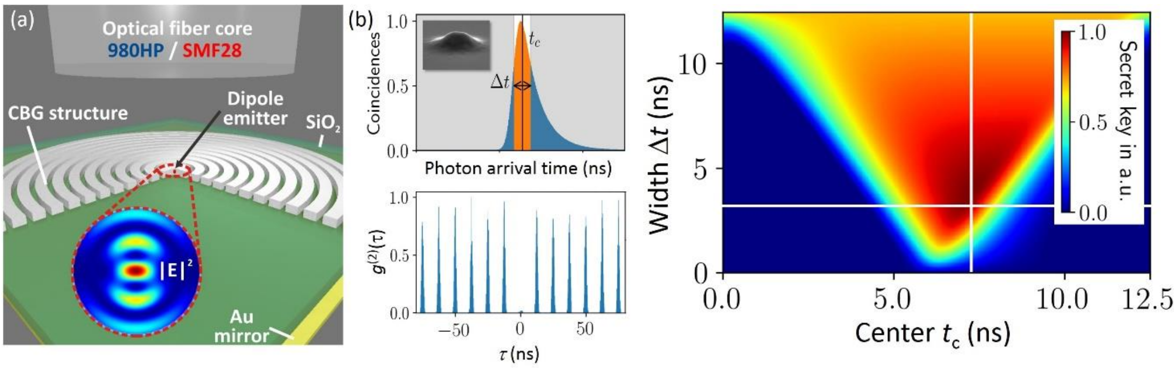

Fig. 1. (a) Illustration of a telecom-wavelength quantum light source based on a hybrid circular Bragg grating device coupled to an optical single mode fiber [2]. (b) Performance optimization of single-photon QKD exploiting 2D temporal filtering using a receiver module developed for polarization encoding [3].

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The virtual lab: Modelling femtosecond nonlinear light-matter interaction

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The cluster of excellence PhoenixD envisions to merge optical systems, design and simulation tools with all relevant production technologies into one combined platform. Essential subtopic is the virtual lab, an ongoing activity to merge different simulation modalities into one multi-scale multi-physics simulation grid.

Abstract

In its current state, numerical optics is well developed, albeit in quite an insular fashion: Thermo-mechanical properties of optical materials can be well calculated, as can light propagation in linear and nonlinear media, or strong field light-matter interaction, and much more. The novel approach and research in PhoenixD is the development of the bigger picture: building bridges and interfaces between the different simulation modalities to realize a platform for modeling and predicting multi-physics and multi-scale systems and processes in optics with high accuracy.

This talk highlights a few examples of femtosecond laser interaction modelling:

- Light accelerates electrons – from Brunel radiation to an optical attoclock [1]; an intensive light pulse ionizes an atom and accelerates the electrons. The collective motion gives rise of the so-called Brunel radiation. Driving the electron with elliptically polarized light on a complex trajectory, the polarization properties of the Brunel radiation reveals attosecond-scale details of the ionization dynamics.
- Light interacts with nano plasmonic antennae – self-optimizing structures [2]; femtosecond light pulses drive plasmonic resonances in planar gold nanoantennas. Gold particles are coldly ablated and transported in the plasmonic field to the high-intensity spots. The deposition of this debris self-optimizes the field enhancement.
- Light controls light – interaction dynamics of incommensurate solitons towards optical transistors [3]; two laser pulses with different colors propagate in nonlinear waveguides in two distinct spectral areas of anomalous dispersion, forming two incommensurate solitons. These two pulses show a rich manifold of propagation dynamics, including robust bound states of light, truly quantum mechanical trapped states in an attractive potential well and analogs to quantum mechanical molecules.

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Contributed talks

Dispersive Quasi Normal Modes (DQNM) in Electrodynamics: Numerical Computation and Modal Expansion

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We present an overview of the numerical computation of Quasi Normal Modes (QNM) in electrodynamics with dispersive materials using the Finite Element Method (FEM). This leads to a non-Hermitian non-linear eigenvalue problem that is numerically solved using the SLEPc library. A very general formula to perform modal expansions of the solutions to scattering problems is displayed.

Quasi Normal Mode Computations

In this paper we present recent developments in our modal expansion technique for electromagnetic structures with highly dispersive media [1]. First of all, the numerical approach requires a robust discretisation of the wave operators associated to the Maxwell's equations. We use the Finite Element Method (FEM) based on edge elements (and their higher order generalizations) that have proved to be spurious mode free. Then a suitable representation of the permittivities as functions of the frequency is provided by rational functions. An interpolation method has been set up that is very accurate on a large range of frequencies and thrifty with the number of poles. The obtained functions are naturally causal (following Kramers-Kronig relations) and provides a natural analytic continuation of permittivities in the complex plane that is necessary for the computation of Dispersive Quasi-Normal Modes (DQNM) associated to complex frequencies (including plasmons in negative permittivity regions). The numerical solution of the Maxwell spectral problems with dispersive media requires efficient non-linear eigenproblem algorithms that are provided by the SLEPc library. In recent versions of this library, our non-linear eigenvalue problems with coefficients that are rational functions of frequency can be tackled directly. Once the DQNM are known, they can be used to perform a modal expansion of the resolvant operator (that can be truncated to a small number of modes for its practical uses). Indeed, despite the fact that the associated operator is non-self adjoint and is a non-linear function of frequency, there exists an exact dispersive quasi-normal mode (DQNM) expansion as we have recently shown using the Keldysh theorem on eigenfunctions of operators depending on a complex parameter [2]. Considering the dispersive Helmholtz equation $\mathrm{T}_{\varepsilon,\mu}(\lambda_s)\mathbf{E_s} = -\lambda_s\mathbf{j}$, the expansion in terms of the right eigenvectors associated with the eigenproblem $\mathrm{T}_{\varepsilon,\mu}(\lambda_k)\mathbf{E_r}_k = 0$ and using the left eigenvectors $\mathrm{T}^*_{\varepsilon,\mu}(\lambda_k)\mathbf{E_l}_k = 0$ for projection is:

$$\mathbf{E_s} = -\sum_{k=1}^{n} \frac{\lambda_s}{(\lambda_s-\lambda_k)} \frac{\left(\int_\Omega \overline{\mathbf{E_l}}_k \cdot \mathbf{j}\, d\Omega\right) \mathbf{E_r}_k}{\int_\Omega \overline{\mathbf{E_l}}_k \cdot \left(\mathrm{T}'_{\varepsilon,\mu}(\lambda_k)\mathbf{E_r}_k\right)\, d\Omega} \tag{1}$$

where $\mathrm{T}'_{\varepsilon,\mu}(\lambda_k)$ the complex derivative with respect to λ_k.

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A high-order accurate, explicit in time, extension of the FDTD/FIT algorithm to triangular meshes

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We present a method that, for the 2D time dependent Maxwell equations, extends the Yee (also known as the FDTD or the FIT) algorithm to arbitrary triangular grids, by using the barycentric dual grid and relating the discrete unknowns for the electric and magnetic fields to edges in the two dual meshes. We show that it is possible to introduce arbitrary polynomial degree in the approximation spaces.

The accurate numerical solution of the Maxwell equations in the time domain, namely

$$\partial_t \varepsilon \boldsymbol{E}(\boldsymbol{r},t) = \boldsymbol{curl}(H(\boldsymbol{r},t)) - \boldsymbol{J}(\boldsymbol{r},t), \quad \partial_t \mu H(\boldsymbol{r},t) = -curl(\boldsymbol{E}(\boldsymbol{r},t)),$$

is of paramount importance for engineering and scientific applications of electromagnetism in the high-frequency range. The celebrated Yee algorithm[1] offers guaranteed $\mathcal{O}(h^2)$ convergence (where h is the spacing of the grid which discretises the physical domain) only when the discontinuities between materials are aligned with the Cartesian axes. The Finite Element Method (FEM) provides a geometrically flexible alternative, but is forced to either use implicit time stepping schemes[2], or to sacrifice the constraint of continuity of tangent components of the electromagnetic field[3].

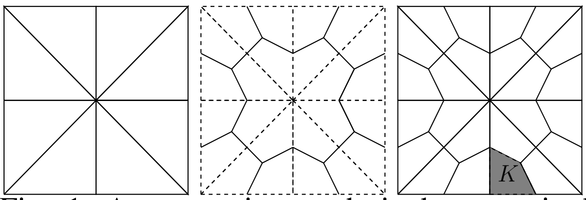

Fig. 1: A toy starting mesh, its barycentric dual mesh, the resulting intersecting cells, e.g. K.

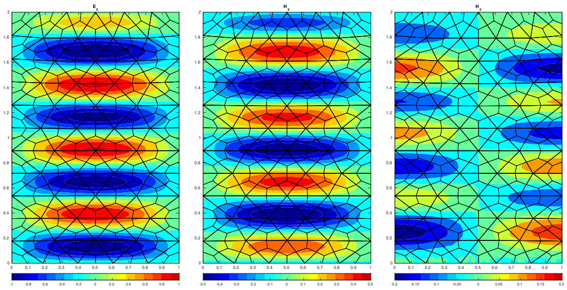

Fig. 2

We propose here a method which overcames both issues: we restrict ourselves to the 2D case in which one of the two fields is a scalar and, relying on the zero-order approach of [4], we approximate the fields inside each K with vector-valued polynomials. The form of the basis functions will be given at the workshop for reasons of space. We anticipate that the resulting method is explicit, spectrally correct, and has optimal convergence rate. As a first numerical result, we show in Fig. 2 the fields due to the dominant mode injected in a slab metallic waveguide of size $a \times 2a$, where a is some characteristic length of the system. The shown snapshot in time was obtained with $p = 5$.

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Beam Propagation Methods for Laser Amplifier Simulation

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There exist different types of laser amplifiers. In particular one has to distinguish amplifiers for continuous wave seed signal, single pulse amplification, and amplification of pulses with low repetition rate or high repetition rate. We present two different simulation techniques for laser amplifiers. The first method models the amplified beam by a set of Gaussian beams. This method can be applied for all types of laser amplifiers and it is less computationally intensive. However, it cannot model a beam distortion of the beam by gain or thermal lensing effects. Such physical effects can be simulated by a beam propagation method for distorted Gaussian beams. Applications of these methods in the commercial code ASLD are presented.

Gaussian beam propagation method

The Gaussian beam propagation method assumes that the seed signal can be modeled by a set of Gauss-Hermite or Gauss-Laguerre functions $E_1, E_2, ..., E_s$. The number of photons of E_k is denoted by φ_k. Now, application of rate equations and transport equation leads to a set of ODE's for φ_k and the discretized population inversion N. The ODE's include overlap integrals of the pump beam and the beam shape $|E_k|^2$. In case of a seed beam of ultra-short pulses with high repetition, a simulation in frequency domain has to be performed (see [1]). However, in case of pulses with low repetition rate, the transport equation has to be solved numerically (see [2]).

The Gaussian beam propagation method is less computationally intensive, but it only allows a rough estimate of the beam quality of the output beam. A more accurate calculation of the beam shape of the output beam requires a beam propagation method (BPM) including a spacial discretization.

Beam propagation method for distorted Gaussian beams

The classical FEM BPM is very computationally intensive in case of beams with a large divergence angle. Therefore, we apply the beam propagation method for distorted Gaussian beams published in [3]. This method applies a factorization of the beam by a low order Gaussian beam TEM_{00} and a smooth unknown factor $\Xi(x, y, z)$ as follows:

$$\Psi(x, y, z) = \Psi_{\text{TEM}_{00}}(x, y, z) \cdot \Xi(x, y, z).$$

This leads to the following equation, which is equivalent to the paraxial approximation of Helmholtz equation:

$$2i\tilde{k}\frac{\partial \Xi}{\partial z} = \frac{\partial^2 \Xi}{\partial x^2} + \frac{\partial^2 \Xi}{\partial y^2} - 2i\tilde{k}\frac{1}{q+z}\left(x\frac{\partial \Xi}{\partial x} + y\frac{\partial \Xi}{\partial y}\right) - (\tilde{k}^2 - k^2)\Xi.$$

Here, $\tilde{k}$ is an average value of the wavenumber $k(x, y, z)$ and q is the complex Gaussian beam parameter. The unknown distortion $\Xi(x, y, z)$ can be calculated by a suitable space stepping method.

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Different Approaches to the Hydrodynamic Material Model within the Discontinuous Galerkin Time-Domain Method

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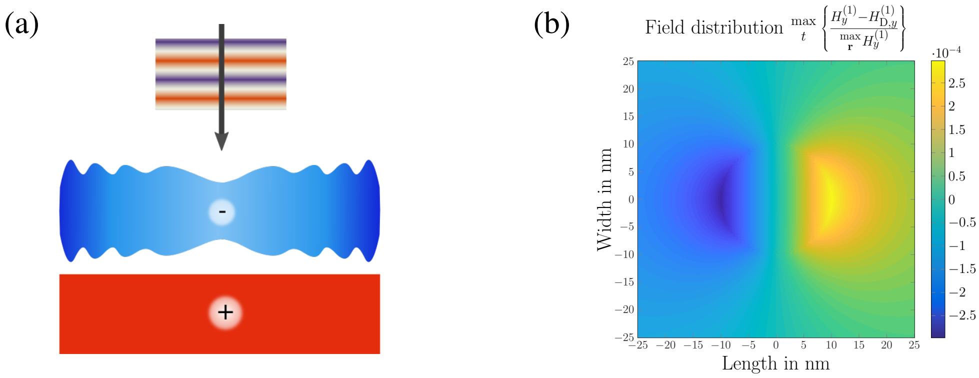
We present a perturbative nonlinear approach to the hydrodynamic material model as well as a linearized approach extended by a drift current density, which are integrated into a numerical discontinuous Galerkin time-domain framework.

Hydrodynamic nano-plasmonics

One popular way to describe plasmonic nano-structures is the hydrodynamic material model – a nonlinear as well as nonlocal model. To anlayze the associated nonlinear effects we find a perturbative approach to the hydrodynamic model to be beneficial as we cannot only clearly separate linear and nonlinear spectra but also display time-resolved nonlinear field information. To this end, we integrate the material model into a numerical discontinuous Galerkin time-domain scheme [1], where the perturbative hydrodynamic material equations are solved alongside with Maxwell's equations. The resulting numerical scheme is demonstrated on a silver nano-wire setup, where we perform three-wave-mixing with two ultra-short excitation pulses. Thereby, we use the setup's resonances to tune the incoming pulses' center frequencies so that the optimal nonlinear output intensity is achieved [2]. As a second approach to the hydrodynamic model we focus on its linearized version but now extend the linear model by introducing an additional drift current density. The result is a hybrid between the original hydrodynamic model for metals and the drift-diffusion model for semi-conductors. We offer some preliminary results on this novel material model.



(a) Sketch of a plane wave excitation of a hydrodynamic metal. (b) Influence of the drift current on a spherical silver scatterer: The response of a silver scatterer is computed numerically for the linearized hydrodynamic material with and without additional drift-current. The difference between these calculations is displayed on the right figure.

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Adjustable Dielectric Metasurface for Enhanced Photon Up-Conversion

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Efficient photon up-conversion under low irradiance conditions is crucial for many applications ranging from bioimaging to photovoltaics. We present large-area dielectric metasurfaces based on silicon photonic crystal slabs and optimize it for selected photon up-conversion applications. By adjusting one single, experimentally easily accessible parameter – the photonic crystal slab thickness – we are able to systematically shift the spectral position of resonances over several hundreds of nanometers. Such resonances are often associated with strong near field enhancement effects. We examine optical near- and far-field characteristics of the dielectric metasurfaces numerically and experimentally. For three typical excitation wavelengths in the near infrared, used for applications in biophotonics (808 nm and 980 nm) and photovoltaics or telecommunication (1550 nm), we determine optimum slab thicknesses. Our simulations reveal up to 17-fold enhanced near field energies at normal incident irradiation, but over 500-fold enhancement at slight oblique incident angles. We explain the limited enhancement factors at normal incidence by forbidden coupling of external radiation with symmetry-protected bound states in the continuum. Slight oblique incidence breaks the symmetry and a much better coupling between external radiation and metasurface is possible. Finally, we demonstrate experimentally enhanced photon up-conversion of $NaYF_4:Er^{+3}$(3%) particles on the metasurface and excited at 1550 nm at slight oblique incidence. These results pave the way for low-threshold photon up-conversion in future solar energy and biosensing applications.

Upper bound of a nanovolume absorption cross-section situated in the vicinity of a nanoantenna

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From first principle calculations, we derive a fully-vectorial upper bound for the absorption cross-section of a nanoparticle situated in the vicinity of a nanoantenna. It is valid for any environment or illumination and it allows to decouple the choice of the environment from the one of the absorber. It provides a meaningful figure of merit to compare the ability of different systems to enhance absorption.

Results and discussion

The absorption cross section of a nanoscale volume V_e filled with a material of dielectric permittivity ε follows this expression:

$$\sigma_{abs}(\boldsymbol{u},\omega) = \frac{\omega}{2P_0}\int_{V_e} Im\,(\varepsilon)|E|^2\, d^3r \qquad (1)$$

where **u** and ω are respectively the direction and frequency of the incident plane wave, P_0 is the norm of its Poynting vector and $|\mathbf{E}|^2$ is the total electric field inside the nanovolume. Generally, the electric field is enhanced thanks to a nanoantenna situated close to the nanovolume. This equation shows that, in order to maximize the absorption cross-section, the product of the dielectric permittivity with the squared field enhancement has to be optimized. Yet these two values are highly correlated and the actual field enhancement in the whole system depends both on the antenna geometry and on the material composing the absorber.

On the contrary the upper bound that we will present for the absorption cross-section solely depends on the complex environment geometry (it is neither the Purcell factor nor the field enhancement but an interplay between two fundamental properties of the environment: the field enhancement $\mathbf{E}_b$ created by the sole nanoantenna and the Green tensor **G**) and thus allow to disentangle the optimization of the nanoantenna from the one of the nanovolume [1]. Therefore, it constitutes a novel figure of merit for comparing the ability of different nanoantennas to enhance absorption. Within the scalar approximation, the upper bound appears to be the ratio between the intensity enhancement $|E_{bz}|^2/|E_{inc}|^2$ and the LDOS enhancement g_{zz}/g_0, with $g_0\mathbf{I} = ½\mu_0\omega^2 \mathrm{Im}[\mathbf{G}_0(\mathbf{r}_0;\, \mathbf{r}_0)] = \omega^3 n/(12\pi\varepsilon_0 c^3)\mathbf{I}$ and $\mathbf{g} = ½\mu_0\omega^2 \mathrm{Im}[\mathbf{G}(\mathbf{r}_0;\, \mathbf{r}_0)]$. Still in the scalar approximation, and for plane-wave illumination, a link can also be made between our upper bound criteria and the gain of an antenna (defined in the classical antenna theory). Our work allows to generalize these existing results, while enlightening the link between field enhancement, LDOS and nanoantenna gain.

This theory will allow to evidence other objects with a far larger upper bound value than the one obtained for dimer plasmonic nanoantenna. In fact, we highlight that, quite counterintuitively, hot spots or resonant objects are not the best choice to maximize the absorption.

Eventually, we will show that our theoretical results can be applied beyond the scalar approximation and the plane wave illumination.

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Causality as Construction Principle for Transparent Boundary Conditions

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Causality in time yields a general construction principle for transparent boundary conditions or field absorbing layers. We discuss a simplified model situation where a signal is generated inside a computational domain at time $t = 0$ and parts of the corresponding field leave the computational domain for times $t \geq 0$. These leaving waves are causal waves. Causal waves have a direct description in Fourier space (as dual to time domain) and can directly distinguished from general, non-causal waves. This gives a framework for analyzing existing techniques like the *Perfectly Matched Layer (PML)* technique as well as for the construction of new algorithms. We discuss this exemplarily based on a 1D model with heterogeneous exterior.

Causality as General Construction Principle

Several approaches are used to treat scattered waves outside computational domains. In numerical practice, PML techniques are used nearly exclusively. We propose the concept of causality to achieve a new understanding of the existing methods, in particular of PML, and to derive new algorithms with extended applicability. The approach is as follows:

1. Space-time domain. We start with the wave equation in space and time, decompose the space into computational domain and its exterior, and consider a signal source inside the computational and define causal scattered waves for any position exterior to the computational domain as a limit condition.

2. Space-frequency domain. Instead to use a single frequency time-harmonic approach, as it is done usually, we apply the formal complete Fourier transform in time restricted to causal waves, both for real and complex extended frequencies. This has the advantage of leaving the initial and boundary conditions intact. At a later stage, we reduce it to a single frequency situation to arrive at the standard setting. The limit equation defining the causality is translated directly into the Fourier domain.

3. Laplace and Laplace-Bloch transform. The causality condition must hold true for any position exterior to the computational domain. To analyze this conveniently, we use either the Laplace transform or the Laplace-Bloch transform in space. The limit equation from item 2 translates directly into a condition of the type: if the limit condition defining causality holds true, the field in Laplace domain must be analytic in a certain complex half-plane of the dual domain. The converse holds also true: If the field in the dual domain to space is analytic, the corresponding space-time solution must be causal.

Algorithmic Demonstration

The concept is neither restricted to 1D nor to a special kind of discretization. For demonstration purpose we use a semi-infinite exterior domain exited at its left boundary with a time-harmonic wave. The refractive index distribution in the exterior domain might be constant, periodic, or even more general. We compute the discrete Dirichlet-to-Neumann operator at the left boundary and compare it to results obtained with the matrix-transfer algorithm.

Benchmarking numerical modal methods for modeling plasmonics structures.

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Popular numerical modal methods devoted to plasmonics structures are benchmarked. A special attention is paid to the spline modal method.

Numerical Modal Methods

Numerical modal methods differ in the choice of expansion and test functions. One can distinguish full domain functions or sub-domain functions according to whether they are defined on the whole domain or only on some part of it. For periodic problems, the most popular method is certainly the well known Fourier Modal Method [1] in which expansion and test functions are pseudo periodic functions. Hence, the various lateral boundary conditions that may arise in the case of structures with different materials and that define the eigenvalue problem are automatically satisfied without writing them explicitly. Although FMM has known many stages of improvements among which the so-called Fourier factorization rules [2], adaptive spatial resolution [3] and the use of symmetries, it nevertheless remains that it converges slowly for structures with permittivity function with negative real part. However, such structures are of common use in modern optics and plasmonics. On the contrary, using sub-domain expansions within each domain that constitute the structure allows to express rigorously the different continuity relations that determine the eigenvalue problem and thus leads to exponential convergence for the eigenvalues and eigenvectors. Our presentation will be devoted to the comparison in term of accuracy and convergence of numerical modal methods as applied to photonic and plasmonic structures. This domain is one for which convergence is the most difficult to obtain and rarely investigated in papers. We will distinguish two kinds of modal methods according to whether they use full-domain or sub-domain basis expansions. In the first set we will consider the Fourier Modal Method,the B-spline modal method [4] and in the second one Pseudo-Spectral modal methods [5] [6] and Polynomial modal methods [7]. In addition, we will present a new algorithm based on B splines which is comparable to spectral elements methods.

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Models for wave propagation in enhanced Kerr nonlinear dielectric media: applications to the spatial control of bulk nonlinearity

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We present two new models to describe the wave propagation in enhanced Kerr nonlinear dielectric media. The first one is a scalar one based on our improved version of the spatial nonlinear Schrödinger equation while the second one is nonlinear FD-TD model that can deal with vector effect and anisotropy. We illustrate their usefulness an complementarity through comparisons with recent experimental data and through innovative devices ensuring a spatial control of Kerr nonlinearity of bulk medium.

We have recently demonstrated plasmon-soliton waves in properly designed multilayered dielectric-metal structure [1]. In order to go beyond this initial work, we have built two new complementary models taking into account the tranverse field profile, the structural inhomogenities along the propagation axis, and also the Kerr type nonlineary of one layer. After their descriptions, we show that as expected the vector model can provide a better quantitative description of the different phenomena but with a much higher computational cost. Then, we use them to show how one can get a spatial control of the effective nonlinearity in properly designed integrated optics devices through the use of plasmonic reinforcement of the Kerr nonlinearity of the bulk layer.
The first model is based on the scalar spatial nonlinear Schrödinger equations (SNLSE) to study the propagation of a beam along a structure with reinforced nonlinearity (see Fig. 1). This model describes the transverse field profile along the Y-axis and its evolution versus propagation along the Z-axis. The field dependency along the vertical X-axis is considered indirectly through the Z-dependent modal properties that appear in the SNLSE. These modal parameters are obtained from the FEM-based nonlinear modal simulations [2] of the different sections of the full structure. The

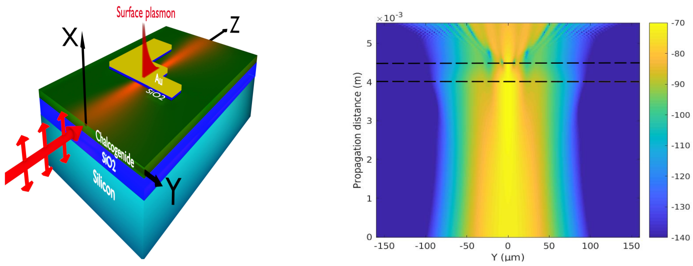

Fig. 1. Left: Scheme of one modelized structure with beam injection and axis definitions, the nonlinear layer is the dark green one. Right: Color map in log scale of the beam intensity evolution along the Y-axis versus propagation inside the full structure for TM polarization with a 500 μm wide gold stripe in the nonlinear regime. The dashed lines represent the limits of the gold stripe.

second model is a 2D nonlinear FD-TD model that can deal with vector effect and anisotropy. It has one dimension for the propagation axis Z-axis and one transverse direction (Y-axis). The included nonlinearity is of Kerr type like in the first model. The crucial point is that it can be inhomogeneously distributed in the structure due to the nonlinearity enhancement ensured by the plasmonic patterns.

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A collection of 3D full-vector finite element models for waveguide-based plasmonic sensors

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The context of this theoretical and numerical study is the design of efficient plasmonic waveguides for infrared sensing [1]. The device configuration is fully integrated and based on a ridge waveguide upon which metallic scattering nano-objects will ensure the coupling between the guided modes and superstrate of the device. Chalcogenide glasses are chosen for the main layers due to their high transparencies for infrared wavelengths. The sensing property relies on the subsequent modification of the guidance of the full structure.

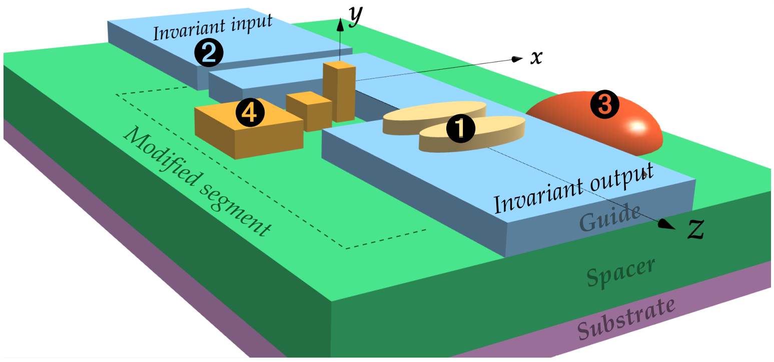

Fig. 1.: Typical waveguide and possible obstacles. Any bounded modification of the permittivity of the invariant structure can be considered: Ellipsoidal patches above the guiding layer ❶, holes ❷ in the guiding layer, obstacles or resonators next to the waveguide ❸ or even a combination of all ❹...

In this frame, we present a general methodoloy to study rigorously discontinuities in open waveguides (see Fig. 1). It relies on a full vector description given by Maxwell's equations in the framework of the finite element method. The discontinuities are not necessarily a small perturbation of the initial waveguide and can be very general, such as plasmonic inclusions of arbitrary shape. The leaky modes of the invariant structure are computed first [2], then serve as incident fields on the full structure with obstacles using a scattered field approach [3]. The resulting scattered field is finally projected on the modes of the invariant structure making use of their bi-orthogonality [4]. A complete energy balance is performed. Finally, the modes of open waveguides periodically structured along the propagation direction are computed. The relevant complex propagation constants are compared to the transmission obtained for a finite number of identical cells. The relevance and complementarity of the two approaches are highlighted on a numerical example encountered in infrared sensing. Open source models allowing to retrieve the presented results are provided [5].

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Epsilon-near-zero Modes of Transdimensional Planar Metallic Nanostructures

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We use macroscopic QED with the confinement-induced nonlocal dielectric response function to study epsilon-near-zero (ENZ) modes coupled to a point dipole emitter (DE) near a transdimentional metallic film. We report the thickness-controlled spontaneous decay with up to three-orders-of-magnitude increased rates.

Abstract: Transdimentional (TD) materials are ultrathin planar nanostructures composed of a precisely controlled finite number of monolayers [1]. Plasmonic TD materials (ultrathin finite-thickness metallic films) offer advances such as thickness-controlled light-matter coupling and new quantum phenomena that can further develop the fields of nanophotonics and metamaterials [1-6]. As opposed to conventional thin film models studied previously that rely on either purely 2D material properties, or on 3D materials with macroscopic boundary conditions imposed on their top and bottom interfaces [7-12], the film dielectric response model we use takes explicitly into account the vertical confinement of charge carriers in the ultrathin TD films. We report new remarkable confinement-induced effects [5]. They are the surface plasmon mode degeneracy lifting and the DE coupling to the ENZ modes split. This coupling leads to the biexponential DE-surface distance dependence of the spontaneous decay with rates two-to-three orders of magnitude greater than in free space. Importantly, these effects can be controlled due to the thickness-dependent plasma frequency of the TD film [2] — a unique microscopic property that cannot be obtained from the macroscopic boundary conditions imposed on the bulk metal film interfaces. The vertical confinement turns the electron-electron Coulomb potential into the much stronger (and thickness-dependent) Keldysh-Rytova interaction potential [13], leading to the thickness-dependent plasma oscillation frequency of the film and thus providing the possibility to control the light-matter interactions, the magnetooptical response, and the near-field properties of the ultrathin metallic films in the TD regime [2-5]. Our results generalize the fundamental work by Drexhage [14] as well as those of related recent work [15] by specifically demonstrating how the light-matter interaction properties in finite-thickness metallic films evolve with their thickness decrease from the bulk material properties to those of 2D plasmonic materials.

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Optimal Photonic Crystal Cavities for Coupling Nanoemitters to Photonic Integrated Circuits

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Photonic integrated circuits hold great promise for realizing scalable quantum technologies. On-chip implementation of those circuits requires an efficient interface between quantum emitters and nanophotonic devices. Such an interface can be provided using photonic crystal nanobeam cavities. Here, it is shown that photonic crystal nanobeam cavities for the visible spectrum can be designed and fabricated directly on-substrate with high quality factors and small mode volumes.

In the last decade, integrated quantum photonics has emerged as a tool to improve the performance of single photon emitters (SPEs) by altering their emission characteristics through integration with nanophotonic devices. The use of optical resonators is especially useful for improving the photon emission rate of SPEs via the Purcell effect. Photonic crystal cavities have shown to be the superior resonator choice for integrated optics as they provide a combination of high quality factors and wavelength-scale mode volumes.
We show that the design and fabrication of photonic crystal nanobeam cavities in the visible wavelength regime is possible directly on-substrate. Our cavities are designed to host NV-centers in nanodiamonds. We stress that the on-substrate design allows compatibility with modern fabrication processes. Three different cavity geometries based on a mode-matching and a deterministic design approach are optimised using 3D-FDTD simulations. After optimization of the photonic crystals band structure in terms of its reflectivity and midgap frequency, we created and optimised the cavities based on the respective design approach. Here, we present our optimization strategies and the resulting parameters. Additionally, we monitored the quality factor of the photonic crystal cavities under geometry variations to analyse contributions of out-of-plane scattering and transmission losses seperately. Finally we verify the theoretical predictions experimentally, finding a reasonable agreement. In our case the mode-matching design is found advantageous for on-substrate realizations.
Our results pave the way for integrating quantum emitters with nanophotonic circuits for applications in quantum technologies.

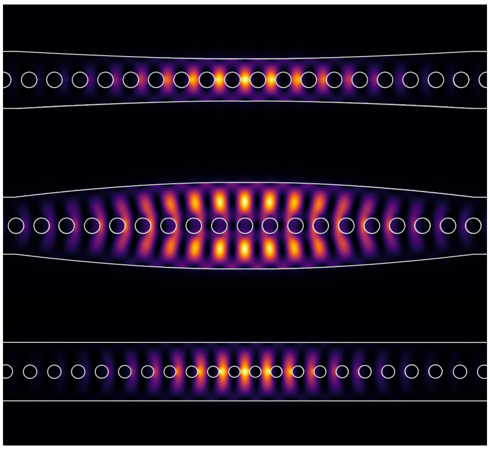

Figure: *Dielectric structure and total electric field density of the three optimised cavity designs. Top and center: quadratic tapering of waveguide width (Deterministic design approach). Bottom: linear tapering of hole radii and distances, additional defect length (Mode-matching design approach).*

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Inverse Design Methods using FDTD for Manufacturable Photonic Devices

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We present a new photonic inverse design method based on an FDTD solver. It automatically generates compact and efficient photonic devices while simultaneously ensuring robustness and manufacturability via commercially available optical lithography.

The design of increasingly complex photonic integrated circuits (PICs) requires the individual components to become more compact, more efficient and more tolerant against manufacturing defects or variations. Photonic inverse design techniques are promising tools which allow designers to directly specify performance targets and manufacturing constraints.

Here, we present our work on the open-source framework ‘lumopt’ [1] which implements a photonic inverse design approach based on the adjoint method [2]. It uses a finite-difference time-domain (FDTD) solver which allows us to efficiently optimize structures over a broad spectral range. In addition to improving the parametric shape optimization offered by lumopt, we added a topology optimization mode which enables the automatic generation of compact, high-performance devices without the need for an initial design idea.

To ensure manufacturability, we demonstrate how to include robustness against over-etch/under-etch as well as the enforcement of minimal feature sizes into the optimization. As an example, we show a novel, extremely compact design of a 4-channel coarse wavelength division multiplexing (CWDM) demultiplexer in the O-band generated using topology optimization (Fig. 1).

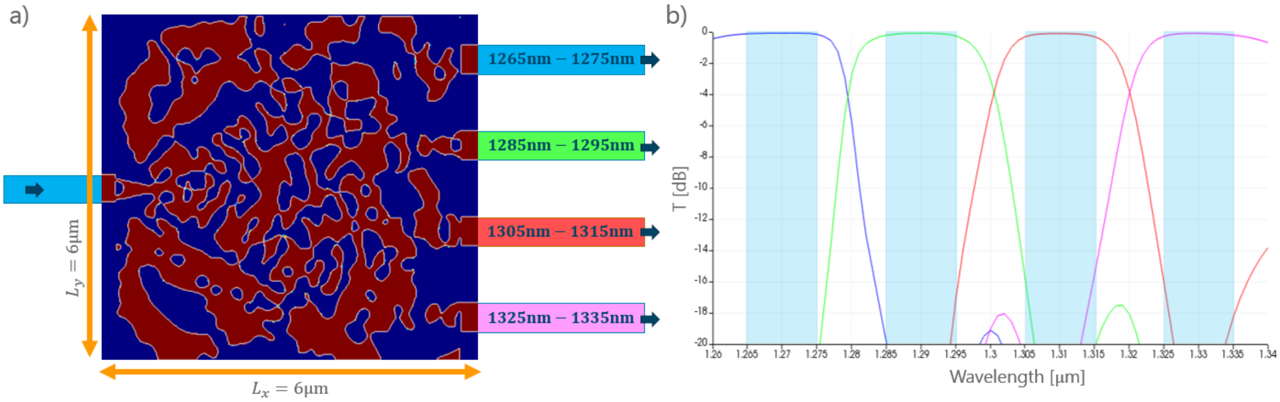

Fig. 1: (a) Result of a topology optimization of a 4-channel CWDM demultiplexer. (b) Corresponding transmission spectra of the four channels.

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Microstar cavities for light confinement without reflection

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We report on a new type of optical microcavities where the light confinement is based on the perfect transmittance at Brewster's angle. In contrast to the traditional microcavities neither total internal reflection nor a photonic band gap is exploited. We rather propose a star-shaped cavity where light rays sequentially leaving and reentering the spikes on a periodic orbit without loss of intensity. Accordingly, in wave optics long-lived modes with fascinating properties arise.

Ray dynamics

If a polarized light ray impinges upon a dielectric interface under Brewster's angle, it is perfectly transmitted. This phenomenon can be used to design a star-shaped cavity with properly adjusted refractive index n such that the rays propagate along periodic orbits as shown in Fig. 1(a). These marginally stable periodic rays are confined without any reflection and they do not lose intensity with time.

Wave dynamics

The wave dynamics is expressed in terms of optical modes being solutions of Maxwell's equations with a (damped) harmonic time dependence. As shown in Fig. 1(b), we verify that the microstar give rise to modes with high quality factors that are supported by Brewster's angle. From the ray dynamics the free spectral range of these modes and their quality factors can be predicted.

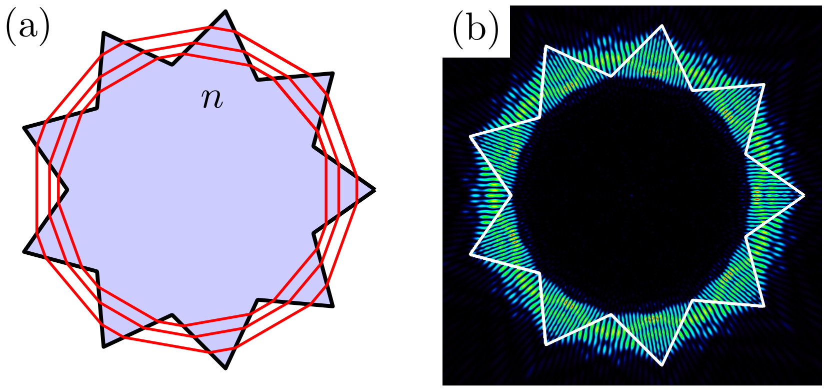

Figure 1: (a) The ray dynamics in the microstar cavity with nine spikes and adjusted refractive index n. In (b) the intensity mode pattern of a long-lived optical mode is shown.

Nonlinear THz wave Transmission Control of Graphene

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We theoretically investigated bistable terahertz (THz) wave transmittance of graphene embedded in thin layers of dielectrics. By solving nonlinear wave equations containing the third order optical nonlinearity of graphene, we numerically observe hysteresis transmission of THz wave through graphene as a function of incident power.

Nonlinear bistable transmission control of light is the one of fundamental operations requested for optical information processing. Furthermore, ultrafast and highly energy-efficient optical bistability at room temperature are required conditions for optical devices [1]. As a new emerging 2D material, graphene has been intensively investigated for its nonlinear optical properties in a broad frequency range from visible to THz waves [2, 3]. In special, strong third order optical nonlinearities of graphene in THz regime have been theoretically explained [4] and experimentally demonstrated [5].

In this presentation, we show that bistable THz wave transmission control with moderate incident power can be possible by embedding graphene in a thin layered dielectric system as schematically depicted in figure (a). Because graphene's nonlinear conductivity is decided by the intensity of the electric field at the graphene position, nonlinear wave equations for THz wave transmitted through the multilayer system must be solved in a consistent manner. In figure (b) THz optical bistability (OB) of graphene on a dielectric substrate (ε_1=ε_3=2.25 and ε_2=ε_4=1) is numerically simulated at 1 THz, where the bistable transmitted power is bounded by the upper (σ_g=0 for no graphene) and lower limit (σ_3=0 for zero optical nonlinearity), respectively. We study the THz OB depending on the Fermi energy of graphene, thicknesses and dielectric constants of dielectric layers, and demonstrate that the critical powers for the up- (P_u) and down-transition (P_d) can be substantially reduced when graphene is surrounded by asymmetric dielectric environment.

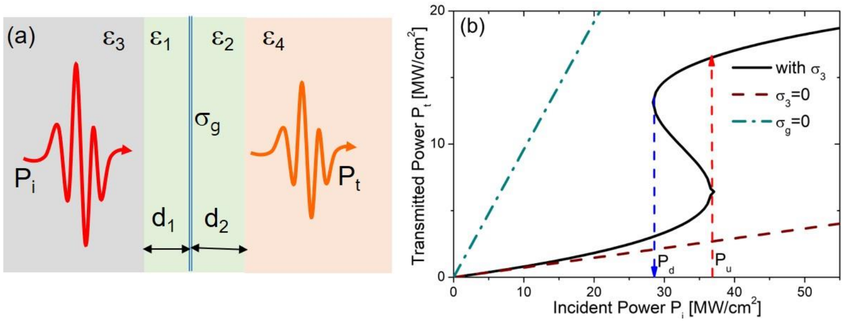

Figure (a) System configuration: graphene embedded in four dielectric layers. (b) THz OB of graphene at the interface between two dielectrics ε_1=ε_3=2.25 and ε_2=ε_4=1 can be obtained at 1 THz with a high Fermi-energy of graphene E_f=1.2eV and is bounded by two limits(σ_g=0 for no graphene and σ_3=0 for zero optical nonlinearity)

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Lossless optical microstrip filters for semi-guided waves at oblique incidence

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A lossless add-drop filter can be realized by evanescently exciting optical microstrip-cavities with a semi-guided wave at oblique angles of incidence. At specific resonance angles, the incoming power is either equally split among all output ports (single cavity) or completely forward dropped to a single port (two cavities).

Single resonator cavity

We investigate optical microresonators consisting of either one or two rectangular microstrip-cavities between upper and lower slab waveguides, separated by a gap g (Fig. 1 (b)). The incoming semi-guided wave of the lower slab waveguide excites the structure at an oblique incidence angle θ (Fig. 1 (a)). Losses are fully suppressed beyond a certain incidence angle [1, 2].

First we examine a microresonator consisting of a single micro-cavity. At a specific incidence angle θ_r, at resonance, the cavity-mode is evanescently excited by the incoming slab mode. The input power is then equally split among each of the four output ports leading to 25% output power at each port (Fig. 1(c)). This resonance angle can be predicted by wavenumber matching of the incoming oblique slab mode and the cavity mode.

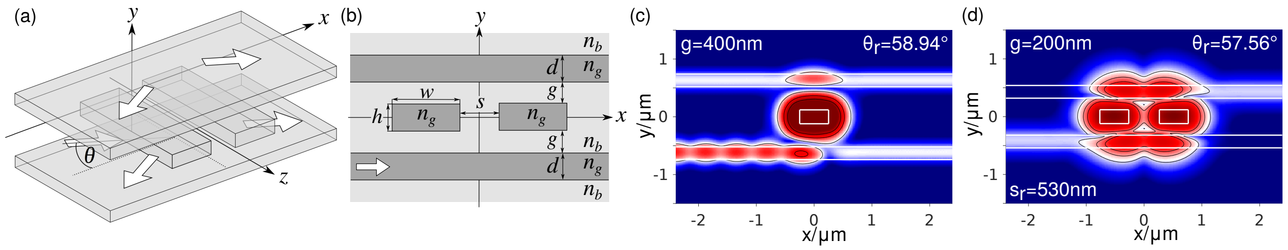

Fig. 1. Oblique excitation of a micro-cavity: 3-D sketch (a), cross section view (b) and field plots of $|E|$ at resonance for one (a) or two (b) cavities with waveguide parameters $n_g = 3.45$, $n_b = 1.45$, $d = h = 0.22\mu m$, $w = 0.5\mu m$, variable gap g and separation s.

Add-drop filter

An add-drop filter can be realized [3] by considering two identical cavities separated by a horizontal distance s (Fig. 1 (b)). For small separations s two cavity modes with even and odd symmetry exist. By exciting the structure at resonance angle θ_r and separation s_r, the modes become degenerate and are excited simultaneously. This leads to full power drop to the forward upper port due to interference in the slabs (Fig. 1 (d)). For increasing cavity distance the system becomes decoupled. Hence, the cavities must be treated as two separate systems, that do not directly influence each other. By exciting the structure under the resonance angle for a single cavity, the mode in each cavity is excited. These modes couple back into the slabs, where the fields interfere. Again, this configuration is also able to route all input power to the forward drop port for specific, large cavity distances s_r. We show that this behavior can also be understood in terms of a semi-analytical model.

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Statistical learning optimization for highly efficient graded index photonic lens

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We present rigorous modeling and optimal design for 3D graded index photonic lens at the telecommunication wavelnegth. Based on our numerical results, the efficiency of the optimized designs can reach 87%.

In this work, we use a global optimization method based on statistical learning in order to enhance the efficiency of a graded index photonic metalens (see Fig. 1(a)). This method belongs to the class of Bayesian optimization methods and is known as Efficient Global Optimization (EGO) [1, 2]. As a 3D fullwave solver, we use our rigorous Discontinuous Galerkin Time Domain (DGTD) solver from the DIOGENES software suite [3] in order to rigorously model such configuration. For the metalens

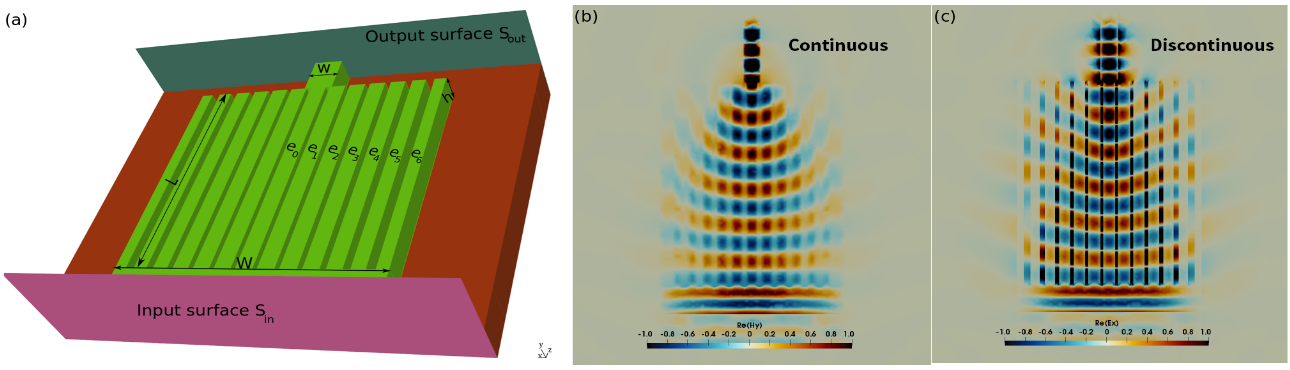

Fig. 1. (a): schematic view of the 3D photonic metalens. The structure consists of Si region (green part) on top of subtrate made of SiO_2 (red part). The Si region is divided into three parts; the input port with width $W = 3000$ nm, the output port with width $w = 300$ nm, and in between we have several Si strips with length L and height $h = 310$ nm. The input mode is injected from the surface S_{in} (solution of the 2D modal problem) and the objective function is computed at the output surface S_{out} as the overlap between the obtained solution and the solution to the 2D modal problem at this surface. The widths of the strips are denoted by e_i, $i \in \{0, 6\}$. (b) and (c) represent the $\Re e(H_y)$ and the $\Re e(E_x)$, of the optimized design, respectively.

presented in Fig. 1(a), we optimize 8 parameters, which are the widths of the strips and their common length L. In addition we focus on the most challenging case, i.e., TE case (unlike other works in the literature, where the classical TM case is considered), where the input field is polarized perpendicular to the strips. In this case, the near field coupling has to be taken into account and a higher order fullwave solver is needed. The optimization results reveal that at least two global designs (different parameters) have been obtained in which the efficiency reaches 80%. Furthermore, we show also that the efficiency may reach 87% in case the lengths of the strips are assumed to be different from each others in our optimization process.

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Slender body theory for plasmonic resonances

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We propose a slender-body theory for calculating the surface-plasmon eigenvalues and eigenmodes of smooth high-aspect-ratio metallic nanoparticles (of otherwise arbitrary shape) and their resonant excitation by incident electromagnetic radiation. Using matched asymptotic expansions, we develop an equivalent one-dimensional model which is straightforward to solve numerically and in special cases furnishes closed form solutions.

Elongated metallic nanoparticles are frequently used in nanoplasmonics, as nano-antennas and biosensors, enabling wide tunability and strong field enhancements [1]. We are accordingly motivated to consider the problem of exciting the localized surface plasmons of a *slender* metallic nanoparticle subjected to either incident radiation or a time-harmonic current density in its external vicinity. Assuming that the particle is deeply subwavelength, we adopt the quasi-static approximation of Maxwell's equations. In this context the induced field can be expanded in terms of the solutions of the so-called *plasmonic eigenvalue problem*, which consists of finding the values (eigenvalues) of the ratio between the inclusion's permittivity and the medium's permittivity, for which there exist non-trivial solutions to quasi-static problem in the absence of any forcing.

In this work we use singular perturbation techniques, namely matched asymptotic expansions in the spirit of slender-body theory [2], to develop asymptotic solutions to the plasmonic eigenvalue problem in the limit of diverging aspect ratio. Specifically, we consider a 3D nanoparticle whose aspect ratio we denote by $1/h$. We show that the permittivity eigenvalues $\mathcal{E}$, associated with the longitudinal axisymmetric modes, scale like $O(1/h^2)$ as $h \to 0$. For that family of modes, we have derived a 1D reduced version of the plasmonic eigenvalue problem,

$$q(s;h) + \mathcal{E}(h)\frac{d}{ds}\left(\mathcal{A}(s)\frac{d}{ds}v(s;h)\right) = 0,$$
$$v(s;h) = \frac{q(s;h)}{2\pi}\ln\frac{g(s)}{R^*(s)} + \mathcal{N}\left(q(\cdot;h)\right)(s),$$
$$+ \textit{ appropriate boundary conditions,}$$

where v represents the axial voltage profile and q the charge density per unit length. Here $\mathcal{A}(s)$ and $R^*(s)$ are the area and conformal radius of the particle's cross section at the position s. The operator $\mathcal{N}$, the function g and the boundary conditions depend on the particle's geometry. We have solved explicitly this eigenvalue problem for a prolate spheroid and a ring with uniform cross-section, and proposed an efficient numerical scheme for straight axisymmetric (otherwise arbitrary) shapes with paraboloidal tips and rings with non-uniform cross-section. In the scenario where the metallic nanoparticle is subjected to an incident plane wave, the above eigen-solutions can be used to obtain asymptotic approximations to all optical quantities of interest.

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Numerical Analysis of Emitter Coupling in Photonic Crystal Cavities using Green's Function

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Coupling of a quantum emitter to a cavity enables many applications in bio-sensing and photonic quantum information. We present an approach to calculate the coupling constant and the Purcell factor in photonic crystal devices from Green's function using the finite element method. With this approach it is possible to calculate the spatial distribution of the Purcell factor, enabling optimized emitter placement. We apply this method to a photonic crystal slab cavity for surface emitter coupling.

Introduction

Coupling of a quantum emitter (QE) to a cavity facilitates the generation of non-classical light. It plays a major role in quantum information applications, such as single photon sources (SPSs) [1]. Coupling of a QE to a photonic crystal (PhC) slab cavity has been shown to be promising for SPSs, due to enhanced spontaneous emission. In the weak coupling regime the Purcell effect describes the enhancement in spontaneous emission rate, governed by the local density of photonic states (LDOS) in an optical environment, i.e. a plasmonic antenna or PhC cavity, resulting in lowered decoherence. With the coupling constant g it can be determined whether the system is in strong or weak coupling and it gives the splitting of energy levels for strong coupling. It can be obtained from Green's function. In order to calculate the Purcell factor, the LDOS is calculated via Green's function as well. Here we show that the LDOS, Purcell factor, coupling constant and the resulting emission spectrum of the QE can be calculated with the finite element method (FEM), solving classical Maxwell's equations, allowing for the description of both weak and strong coupling regime of the emitter-cavity system.

Methods and Results

Assuming an emitter with electric dipole transition an inhomogeneous wave equation for the Green's function can be obtained, which is solvable with the FEM. We solve the eigenvalue problem of the cavity, obtaining the complex eigenvalues and electric mode profile. With these results the electromagnetic Green's function can be calculated using a mode expansion approach [2]. From the complex eigenvalue the resonance wavelength and Q factor are calculated.

With the Green's function the spatial distribution of the Purcell factor, as well as the coupling constant and the normalized spectrum of the emitter at a certain position can be determined. The Purcell factor is independent of the QE, as it gives the ratio of spontaneous emission rate and is governed by the LDOS. The coupling constant however depends on the QE as well. Nevertheless with this approach little knowledge of the emitter is needed; the dipole moment, non-radiative decay rate and emission wavelength are sufficient. We will calculate and present the parameters as well as the spontaneous emission spectrum for a surface emitter coupled to a PhC slab cavity.

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A machine learning method for efficient design optimization

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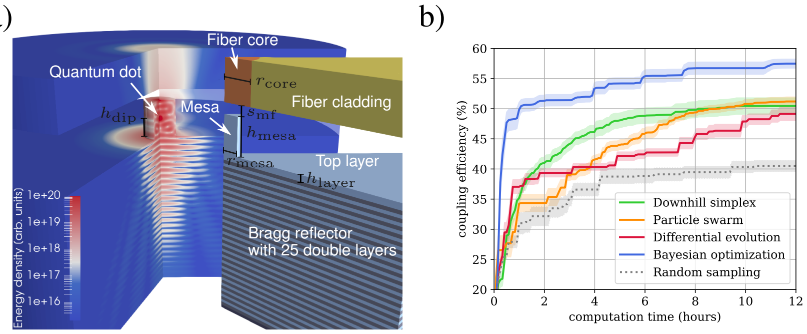
Shape optimization of nano-photonic devices can be computationally very demanding and requires the use of efficient optimization algorithms. We study the performance of Bayesian optimization, which is based on a stochastic model of the objective function.

Numerical optimization is a fundamental task for many scientific and industrial applications. In nano-optics it is applied, e. g., for the optimization of lithographic masks [1] or for scatterometric shape reconstruction [2]. The computation of the objective function often requires to rigorously solve Maxwell's equations for multiple frequencies or incoming light-field directions while the parameter space can consist of ten or more degrees of freedom and contains in general a large number of local extrema. This makes numerical optimization in nano-optics very demanding and time consuming.

We demonstrate that Bayesian optimization (BO) can significantly speed up optimization in nano-optics. BO uses previous evaluations of the objective function in order to train a stochastic model [3]. The model, a Gaussian process, is subsequently used to derive promising parameter values by means of Bayesian inference. In contrast to other local or stochastic optimization methods, this search strategy uses data on *all* previous function evaluations. We demonstrate the advantages of the method by benchmarking BO against other commonly used optimization methods, such as the downhill simplex algorithm, particle swarm optimization and differential evolution [4].

a) b)



a) *Visualization of the light field intensity of a fiber-coupled single-photon source, which is optimized w.r.t. the depicted parameters (black).* **b)** *Average of the best seen coupling efficiency for different optimization approaches versus the total computation time.*

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Simulation of Metasurface Enhanced Photon Up-Conversion

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We present simulations detailing the enhancement of photon up-conversion processes in nanoparticles due to increased local field intensities. The local field enhancement is provided via a photonic crystal slab. Such systems have promising applications in both photovoltaics and bio-photonics.

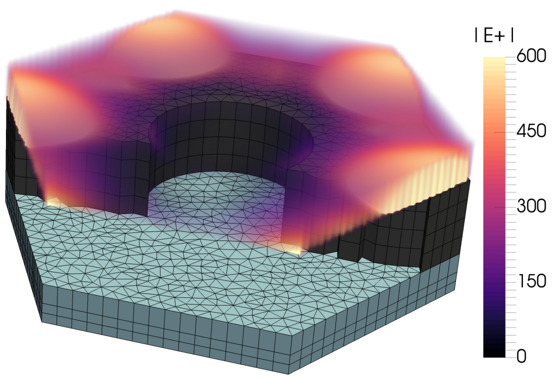
Photon Up-Conversion

The photon up-conversion process describes the absorption of two photons at a certain frequency ω_1 and re-emission of a single photon with a higher frequency $\omega_2 > \omega_1$. This can be applied to increasing the range of the solar spectrum that can be harvested via photovoltaics [1], or for enhanced detection of fluorescence from bio-molecules [2].

Due to the requirement of absorbing two photons, the process strongly scales with intensity. In order to make this process happen efficiently, the intensity of the excitation field in the vicinity of the nanoparticles should be increased as much as possible.

One possible method to accomplish this intensity enhancement is with photonic crystal slabs. These periodic modulations in a dielectric layer support modes traveling in the plane of the slab. In certain cases, these modes couple to external radiation and are typically referred to as leaky modes. This coupling allows the modes to be excited from an external light source, as long as it fulfills the frequency, angle and polarization conditions of the mode in question.

We present calculations of the mode structure of such a photonic crystal slab with and without a nanoparticulate coating. By determining the enhancement in the local square of the intensity we are able to accurately model the up-conversion enhancement seen in experiments.



The enhanced intensity of light in the near field of a photonic crystal slab due to the presence of a leaky mode. Part of the FEM mesh used for simulation of the unit cell is also shown.

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Light-management in nanotextured perovskite solar cells

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Perovskite has recently emerged as a good alternative to silicon for solar cells. Nano-texturing of the perovskite layer in such solar cells could yield a better light-confinement inside the perovskite layer and decrease the reflection of light at the interfaces. This would eventually lead to a higher power conversion efficiency in the solar cell. In this talk, we will present our numerical and experimental studies of perovskite solar cells. In particular, we investigated the role of a sinusoidal nano-texturing of the perovskite layer on the light-absorption and reflection by the solar cell.

Crystalline silicon solar cells are wide-spread due to their large power conversion efficiency and their low manufacturing costs. However, perovskite appears as a good alternive to silicon and tandem solar cells made from both silicon and perovskite have recently been proposed as a promising platform to overcome the theoretical limit of silicon solar cells [1]. Nanotexturing of the different layer interfaces inside the solar cells is also a good strategy to enhance light absorption and the power conversion efficiency of solar cells. Sinusoidal nanotexture have recently been shown to increase light-absorption in silicon and tandem silicon-perovskite solar cells [1, 2].

Here, we present our experimental and numerical study of light management in perovskite solar cells. We compare light absorption in perovskite cells with a planar and sinusoidal interfaces. Numerical simulations are carried out by solving Maxwell's equations using a time harmonic finite element solver (JCMsuite) [3]. The planar solar cell configuration is simulated as a one dimensional multilayer stacks. Solar cells with a two dimensional sinusoidal texture are modeled by a rhomboid unit cell with periodic boundary conditions. We show that a sinusoidal texture with an amplitude of roughly 400 nm and a period of 750 nm can allow for an increase of the optical absorption inside the perovskite compared to the case of planar solar cell. This increase can be larger than 10 percents in some region of the spectrum. A larger photocurrent density is also observed in sinusoidal solar cells compared to planar solar cells both in numerical simulations and experimental measurements.

Acknowledgements

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Engineering asymmetric coupling in two-mode nanostructured dielectric waveguides

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In this work, we study optical properties of dielectric periodic waveguides that possess two modes with identical frequencies and wavenumbers and characterized by different symmetry with respect to the plane that contains the waveguide axis. Our numerical simulations predict that the field pattern of the wave excited in such a waveguide with a circularly polarized point dipole is highly asymmetric and remains in such state during propagation along the waveguide for distances up to several centimeters. We also demonstrate that one-dimensional array of coupled two-mode waveguides exhibits nontrivial topological properties and support topological edge states even with a single waveguide in a unit cell.

Tailoring the spatial distribution and polarization of electromagnetic fields in the near-field zone plays a major role in many nanoscale optical effects, that originate from the interaction between optical nanostructures and quantum emitters (QE), placed in their very proximity [1, 2]. For instance, a simple homogeneous single mode optical waveguide exhibits non-zero local transverse spin density, which leads to the spin-momentum locking, when the direction of light propagation becomes strongly coupled to the polarization state of the source [2]. Such chiral light-matter interaction attracts a lot of interest during last years due to the promising applications in nanophotonics and quantum optics [3].

Here, we consider optical properties of specially designed periodic dielectric waveguides with degenerate modes that can interfere in the near-field zone and lead to highly asymmetric field patterns of the propagating wave [4]. Numerical simulations show that a circularly-polarized QE can unidirectionally excite both modes of the designed nanophotonic waveguide at the same time. This results in the possibility of encoding the polarization state of a QE into the near-field distribution of the propagating optical signal and its transferring for distances up to several centimeters.

As an extension of the proposed idea we show that the designed two-mode waveguide can serve as a building block for topologically nontrivial photonic structures with simple lattice geometry. To that end we consider a one-dimensional array of equally separated identical two-mode waveguides. Our theoretical and numerical analysis reveals that the presence of two modes gives rise to modulation coupling in the array of such waveguides and consequently to the emergence of topological edge modes. We show that such system can be described as a generalized paradigmatic Su-Schrieffer-Heeger model, reducing to it for the suitable parameter choice. We also discuss a feasible experimental procedure that allows for excitation and detection of the predicted edge states in far-field by appropriate polarization of the incident beam.

Acknowledgements

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Triplet fusion photon upconversion materials: a playground at the intersection of photonics and photochemistry

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Triplet fusion is a photochemical process in which two quanta of electronic energy are combined within a single chromophore. When implemented in a suitable material system, triplet fusion enables photon energy upconversion – the emission of photoluminescence with a considerable anti-Stokes shift (of the order 1eV) with respect to the photoexcitation source [1]. The process begins with the optical excitation of spin-1 (triplet) excitons, via a triplet sensitizer material; then the transfer into and diffusion throughout a so-called annihilator material. Triplet-triplet encounters within the annihilator lead to triplet fusion, the resulting high-energy state can then relax via photoluminescence, or energy transfer to a reaction center. Photon upconversion has technological applications in photovoltaics, artificial photosynthesis, imaging, and phototherapies [2].

Photonics plays a significant role in determining photon upconversion efficiency. The process benefits greatly from light concentration, which can be achieved through micro-optical elements or photonic structures, improving the yield of the nonlinear triplet fusion process [3]. An added benefit from thinning the absorbing material is a potential reduction in lossy reabsorption of the upconverted signal. Manipulation of the local photonic environment can also improve the efficiency with which upconverted photoluminescence is extracted from the material bulk, increasing the external quantum efficiency. Compared to the production and characterisation of new triplet fusion upconversion materials, the implementation of these photonic effects has received comparatively little attention.

In this work, we present a review of recent work in the triplet fusion upconversion space, with a focus on recent developments amongst a largely-untapped set of opportunities for the photonic augmentation of photon upconversion. We argue that a holistic view of both the photonic and the photochemical aspects of photon upconversion is vital for obtaining the best possible upconversion performance. The beginnings of such a model will be described.

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An ambient condition nanoscale electrochemic device with direct optical antenna feedback

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We have developed a system of two parallel electrically connected gold nanorods with unequal length and resonances, placed at a short distance of 150 nm. Time dependent white light spectroscopy shows that the humidity of ambient air is sufficient to support electrochemistry when voltages of up to ±20 V are applied. Electrochemical processes reveal themselves by shifts of the nanorod resonances up to 10 nm with a slow time constant on the order of 10 seconds. When the same experiments are performed under a N_2 atmosphere, resonance shifts nearly completely vanish.

Background

It has been shown that small resonant plasmonic nano particles can be tuned by applying a voltage, when placed in an electro-chemical environment. Resonance shifts can occur due to double-layer formation, surface chemistry or charging which are notoriously difficult to distinguish.

By means of two electrically connected antennas (see Fig. 1a)) with out a conductive link in 150 nm distance, we have developed a new system to examine the possible origins of plasmonic resonance shifts. Since the antennas show different resonances (see Fig. 1b)) we can monitor the impact of positive and negative applied voltage in parallel.

We find that the change in resonance happens on a time scale of several seconds, much slower than expected by a purely charging effect. By performing the identical experiment in pure nitrogen atmosphere we can make the resonance shift vanish nearly completely and, thus, prove an electrochemical origin, enabled by the ubiquitous hydration layer on every surface in ambient conditions.

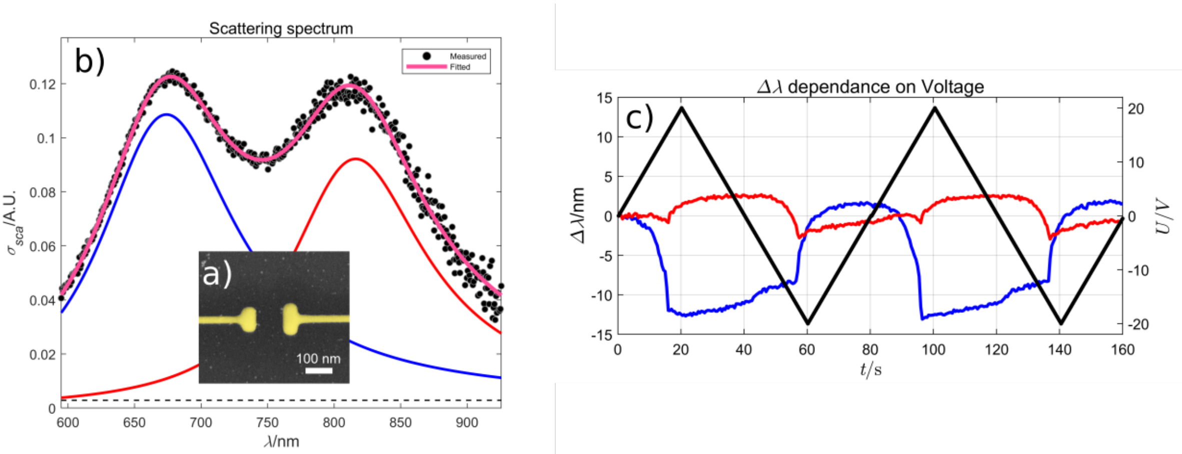

Fig. 1. First results of the device: a) SEM image of the geometry; b) white light scattering (black dots) and fit of the two resonances (blue and red curves) of the structure in a) without applied voltage; c) Applied voltage (black curve) and corresponding measured changes $\Delta\lambda$ in both antennas resonances in ambient conditions. Not depicted are the vanishing curves for the same measurement when performed in a N_2 atmosphere.

Imaging chiral structures: Polarization dependent time- and frequency resolved spectra of photosynthetic complexes

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The specific excitonic energies and the orientation of transition dipole moments in photosynthetic complexes are revealed by varying the polarization sequence of 2D-echo spectroscopy. We discuss the theory behind the experiments and how the optical response function is affected by slight structural changes in the molecular complexes.

Two-dimensional spectroscopy probes the third-order linear response function and yields time- and frequency resolved spectra of energy transfer processes. The response function results from 4 delayed laser pulses interacting with the molecule. For instance in photosynthetic complexes, the energy is efficiently guided from the antenna pigments to the reaction center. On the theoretical side, this requires to include the vibrational modes of the molecules in the description to obtain a spatially directed energy transmission. We have developed theoretical methods and implemented them within the hierarchical equation of motion (HEOM) method, suitable for the energy ranges and physiological parameters found in photosynthetic molecules. In the talk I focus on the impact of varying the polarization of the pulses to infer structural information about the pigments, for instance chirality.

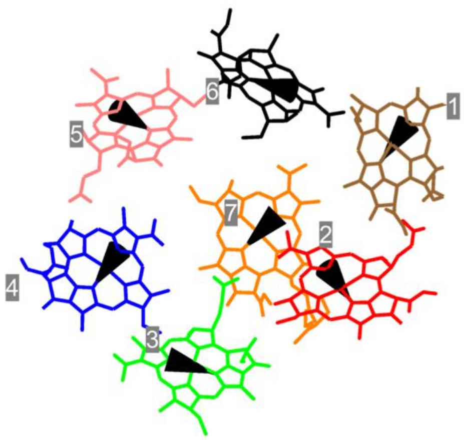

Fig. 2 The orientations of the transition dipoles in the Fenna-Matthews-Olson complex (FMO monomeric unit 3ENI) along the N_B and N_D nitrogens.

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3D Imaging of Vibrational Surface Modes in a single MgO Nanocube

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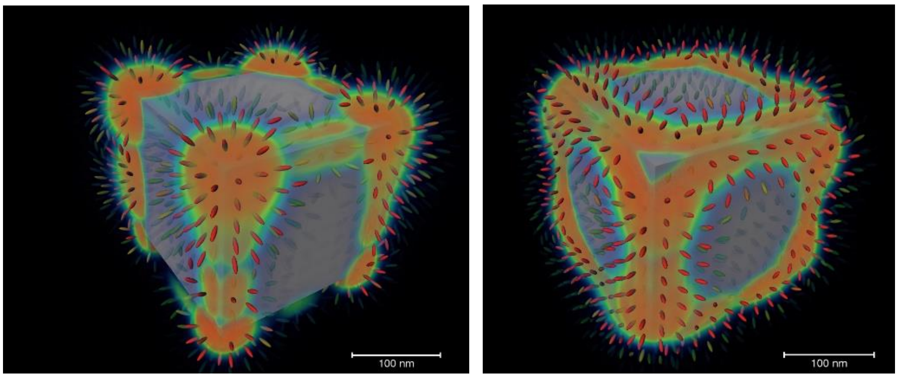
Electron energy loss spectroscopy (EELS) allows imaging of surface plasmon and phonon modes with nanometer spatial and meV energy resolution. Here we present a combined experimental and theoretical scheme for 3D tomographic imaging of the vibrational surface modes of a single MgO nanocube.

Electron energy loss spectroscopy (EELS) has become a key player in the field of plasmonics and nanophotonics [1] as it allows imaging of optical nearfields with nanometer spatial and high energy resolution. With the newest generation of electron microscopes, the energy resolution can be pushed to the meV range thus allowing the direct measurement of surface and bulk phonon modes in ionic nanostructures [2].

In this paper I discuss our recent efforts to combine such high-resolution EELS measurements with plasmon tomography schemes [3], in order to obtain full 3D maps of the nanophotonic environment. Within the near-infrared regime one can safely employ the quasistatic approximation and use the geometric eigenmodes [4] as basis modes for the tomographic reconstruction. For a MgO nanocube I will demonstrate the applicability of the approach in order to map out corner and edge modes. The results will be compared with detailed boundary element method (BEM) simulations obtained with our homemade MNPBEM toolbox.

From our analysis we can identify a number of important ingredients that have been ignored in previous studies, and which can be traced back to significant mode mixing in presence of substrates and difficulties associated with different cluster points for edge and face modes. I will comment on extensions of our scheme for larger nanoparticles using quasinormal eigenmodes, which can be readily computed within our BEM approach.



Tomographic reconstruction of photonic LDOS for corner (left) and edge (right) modes of a single MgO nanocube. The scale bar is 100 nm.

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Material reparametrization for topology optimization of 3D photonic nanostructures

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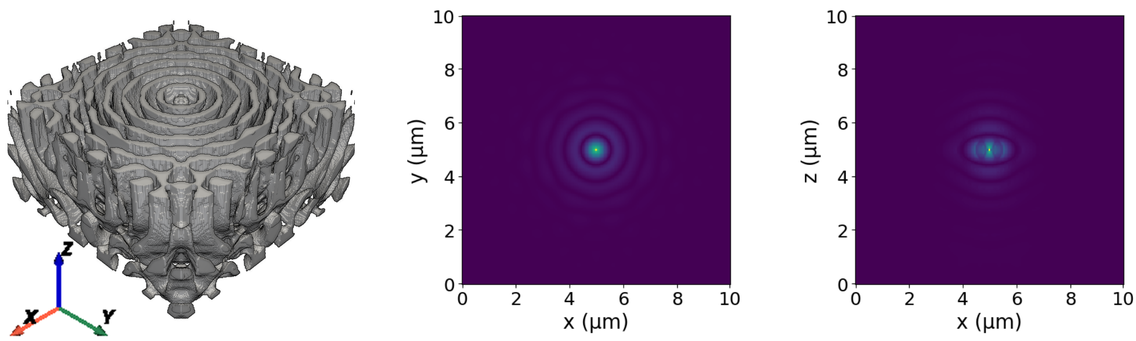
Topology optimization is an inverse design method which can generate nanophotonic devices with optimized material distributions without any constraint on geometrical shapes. Here, we present our recent efforts in the topology optimization of fully 3D nanostructures with an emphasis on challenges and advancements in material parametrization using e.g. neural networks.

Topology optimization in nanophotonics

Local optimization of arbitrary permittivity distributions is made possible by adjoint sensitivity analysis, which enables the efficient calculation of gradients of some objective function F with respect to any number of design variables ρ. The ability to derive gradients w.r.t an arbitrary number of design variables with only two simulations has led to a boom in inverse design in photonics[1]. Much recent research has been conducted with great success on the topology optimization of planar structures for e.g. photonic integrated circuits. This is largely due to practical constraints, but with advancements in multiphoton lithography, fully 3D devices are becoming feasible for fabrication. In this work, we discuss challenges of 3D topology optimization for photonic devices such as structural integrity and design parametrization and present our recent efforts in optimizing such devices (Fig. 1).



(a) Permittivity (b) $|\boldsymbol{E}|$ (x-y plane) (c) $|\boldsymbol{E}|$ (x-z plane)

Fig. 1.: A 3D topology-optimized optical cavity with a resonance wavelength of $1.5\,\mu\mathrm{m}$ and a refractive index contrast of $\Delta n = 0.6$. The designable area consists of a cube with a volume of $10\,\mu\mathrm{m}^3$. Shown is (a) a cross section of the permittivity distribution centered in the x-y plane as well as the absolute electric field at the cavity center in the (b) x-y and the (c) x-z plane.

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Poster presentations

Advantages and limitations of different modeling approaches for characterization of emission of light from III-V nanowires

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Unlocking the huge potential of nanowire-based devices requires accurate characterization and numerical calculations to further enhance their efficiency. In this work, we introduce two possible ways of modeling light emission of a system containing a nanowire (NW), using the COMSOL *Multiphysics* simulation software environment [1], and analyze the magnitude of the parasitic absorption that may occur in a transparent conductive oxide (TCO) top contact layer of the NW structure (see Fig. 1a) and the enhancement factor of the emission rate.

We consider light emission from a NW with two different modeling methods: 1) a method with an actual emitting dipole inside the NW, and 2) a method based on the Lorentz reciprocity where the response to an incident plane wave yields the corresponding far-field emission from a dipole in the NW. The simulations were performed using COMSOL *Multiphysics*, where the finite element method (FEM) is used for solving Maxwell's equations for the diffraction of light by the NW. We compare the results from these two numerical methods to reveal the advantages and disadvantages of each method. The thickness of the TCO layer can significantly affect the total emission rate from the system; that is, it can modify the Purcell factor. Based on our simulation results, we analyzed the absorptance in the TCO layer and how the emission to the top and bottom directions can be managed by varying the parameters of the TCO. Fig. 1b represents, as a function of the TCO thickness, the dependence of the far-field emission to the top and bottom sides from the NW, as well as the absorptance in the TCO.

a) b)

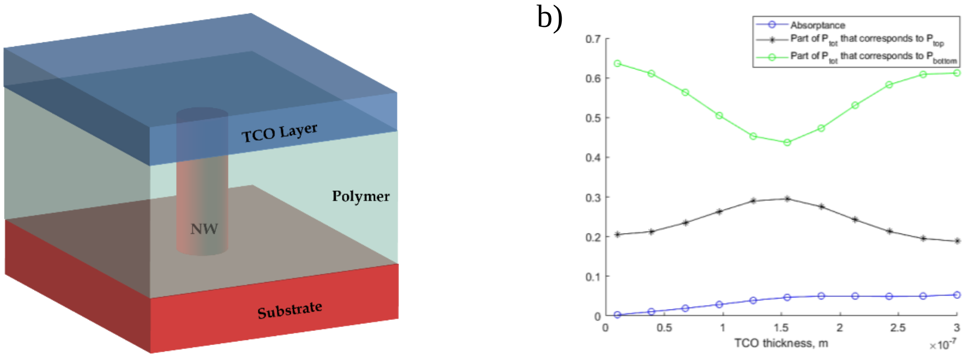

Fig.1. (a) Schematic of the modeled system containing the TCO layer as a top contact. (b) Absorptance in the TCO and far-field emission to the top and bottom sides as a function of TCO thickness.

Comparison of the modeling results will provide a more complete picture of the efficiency and suitability of the different approaches for the modelling of light emission from semiconductor NWs. The analysis of the effect of the TCO on the total emission rate can contribute to a better understanding and improvement of the performance of the manufactured nanowire-based light-emitting sources.

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Grazing incidence X-ray fluorescence measurement on nanostructures for element sensitive reconstruction

Anna Andrle[1], Philipp Hönicke[1], Philipp-Immanuel Schneider[2], Yves Kayser[1], Martin Hammerschmidt[2], Sven Burger[2,3], Frank Scholze[1], Burkhard Beckhoff[1], and Victor Soltwisch[1]

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The production of the current and next generation of semiconductor devices requires a reliable and non-destructive characterization of the material composition and dimensional parameters of the nanostructures is necessary. A method based on grazing incidence X-ray fluorescence measurements is applied to lamellar gratings made of Si3N4. This technique is based on the X-ray standing wave field, which is sensitive to both the elemental composition and dimensional parameters of the nanostructures. With a finite element Maxwell solver, the X-ray standing wave field can be calculated and used in conjunction with a parameterized nanostructure to model experimental data and thus, derive the spatial distribution of elements and the geometric shape with subnm resolution. This reconstruction is executed with a Bayesian optimization approach to minimize the computational effort.

Numerical modelling of second harmonic generation in large subwavelength-patterned highly resonant structures

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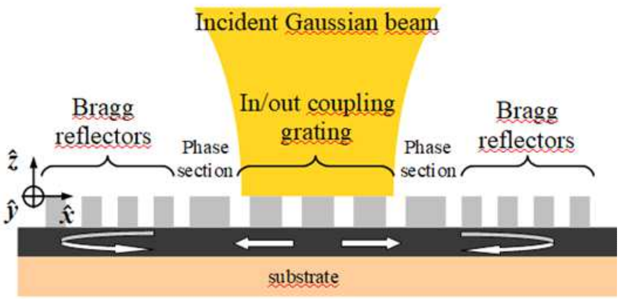
Cavity Resonant Integrated Grating Filter (CRIGF) are promising structures composed of a grating coupler (GC) surrounded with two Distributed Bragg Reflectors (DBR)[1]. The excitation of an eigenmode of the structure through one diffraction order of the GC generates a resonance peak in the reflectivity spectrum, that can reach 90% for incident focused beam ($\simeq$10 wavelengths diameter at waist). We intend to take advantage of the field enhancement caused by the excitation of a confined mode with a focused beam in CRIGF to improve the efficiency of nonlinear optical effects, especially Second Harmonic Generation (SHG). Yet, CRIGF are large ($>$100 wavelengths), highly resonant components, patterned at the subwavelength scale, and their modelling is not trivial. We recently showed the successful modelling of a CRIGF, composed with linear material only, with four different methods (Fourier Modal Method, also known as Rigorous Coupled Wave Analysis, Finite Element Method, Discrete Dipole Approximation, Finite Difference Time Domain Method) [2]. The subject of the present work is the numerical modelling of SHG in CRIGF using the Fourier Modal Method, the Finite Element Method and the Discrete Dipole Approximation. We will detail the modelling principles and show numerical validation in the case of a 2D CRIGF (invariant along y direction, see fig.).



Representation of a CRIGF structure.

Funding Information

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Sub-wavelength Metamaterial for a Variable and finely Tailored Coupling Coefficient within Waveguides Arrays

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Within Silicon-based waveguide arrays, we propose that sub-λ, below band-gap metamaterial can provide variable coupling coefficient with a tailored control and a fine tuning, both for a transverse or a longitudinal coupling variation.

In arrays of coupled optical waveguides, efficient and versatile operation is achieved through an accurate control of the coupling coefficient C. For example, a chirped-transverse coupled array provides 75dB optical isolation ratio for an integrated isolator on Si [1], a variable longitudinal coupling allows adiabatic transfer in a three-core directional coupler [2].

The sub-λ metamaterial can be either 1D, e.g. lines or 2D e.g. holes operated far below its photonic gap. Its optical index can thus be modelled as an homogeneous uniaxial material, whose ordinary and extraordinary indices can be calculated following [3]. We have investigated the relevance of this homogenization approach benchmarking it with 3D FDTD calculation. While the homogenization represents correctly the 1D case (lines) for an electric field parallel to the line, a ~7-10% discrepancy is obtained for E being normal to the lines. This discrepancy is thus found again for the 2D case (holes) having interfaces parallel and normal to E. Additionally, as pointed out in [4], the sub-λ material has to be extended on both sides of the outer guides of the array by adding arms to manage the higher order modes existing in the high coupling sub-λ duty-cycles.

Propagation simulation is performed by the Coupled Mode Theory. For a transverse variation of C, we have calculated the propagation in a 13-waveguide array for Fig.1 (a) constant C, (b) C+ΔC (c) chirped C. Increasing C reduces the device size, the chirped coupling providing the correct bouncing without border jeopardization. For a longitudinal variation of C, the variable duty-cycle of the 1D metamaterial provides the accurate C(z) for the adiabatic transfer. Fig.2 shows (a) the simulated geometry and (b) the optical power versus propagation length on each waveguide.

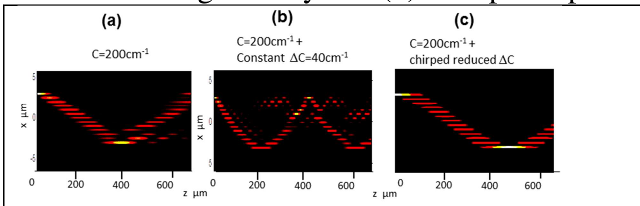

Fig. 1 : Intensity distribution over a 13-waveguide array (a) constant C=200cm-1 (b) variable C C=200cm^{-1} + 40cm^{-1} (c) chirped C =200-195-185-169-148-107 cm^{-1}

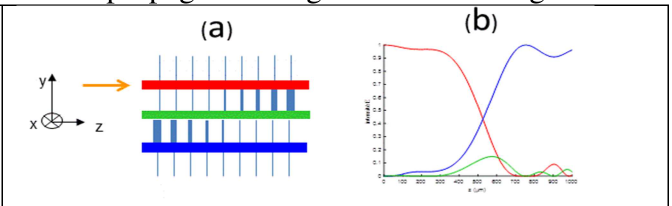

Fig.2 (a) Schematic of the 3-core coupler with variable duty-cycle lines and external arms (b) Optical power versus propagation length, on a 1mm long coupler

Preliminary measurements have been obtained on fabricated arrays on SOI.

We propose sub-λ, below band-gap metamaterial coupled waveguides for accurate and tailored control of the variable coupling coefficient.

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Quasinormal mode expansion for nonlinear optical generation in subwavelength resonators

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We propose an alternative to the multipolar expansion for studying nonlinear processes in optical nanoantennas. Subwavelength resonators can be studied as non-Hermitian open cavities, whose eigenstates are called quasinormal modes (QNMs) [1]. Based on this theory, we derive a novel approach enabling a deep analytical insight into the multi-parameter design and optimization of nonlinear photonic structures at subwavelength scale. A key distinction of our method from previous formulations relying on multipolar Mie-scattering expansions is the exploitation of the natural resonant modes of the nanostructures, which only depend on its geometry regardless of external excitation configuration. We enforce in this work at least two main advantages: (a) the usage of a numerical tool reducing computational costs and providing a deeper physical understanding, and (b) an analytical expression of modes excitation coefficients and mode spatial overlap bringing out phase matching conditions in leaky nanoresonators. Based on the presented formulation of nonlinear overlap integral we introduce a new design pathway for $\chi^{(2)}$ nanoresonator enabling more than two-order of magnitude enhancement for second harmonic generation efficiency [2].

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Photonic Microring Resonators for Temperature Sensing – Multiphysics Modeling and Material Comparison

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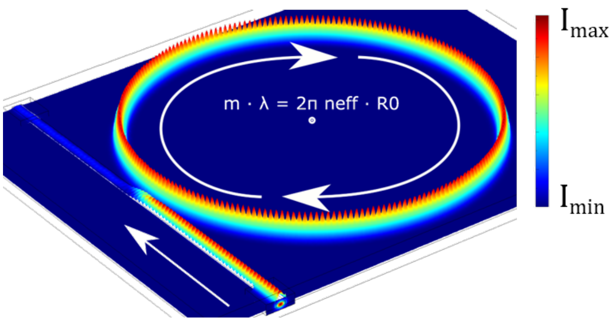
We study the influence of material properties on temperature sensitivity and thermal behavior of photonic microring resonators. To this end we perform simulations based on finite element analysis for the temperature dependent resonance shift and analytic computations to quantify effects like self-heating.

Formatting guidelines

Temperature measurements play an important role in a large variety of application fields ranging from fundamental research to industry and medicine up to everyday life. Particularly the rapdily growing field of quantum technologies requires control of very delicate processes and thus also devices to measure temperature and temperature flows with high spatial resolution and high precision. Photonic microresonators with high optical quality factors are a promising platform for robust high-precision temperature measurements. In this contribution we study the temperature sensitivities of microring resonators made of materials (silicon, germanium and gallium nitride and diamond) with different thermo-optical characteristics at the telecommunication wavelength of 1550 nm. We design the structures with finite element analysis (COMSOL Multiphysics). In addition, we explore the influence of self-heating induced by two-photon absorption on the accuracy of temperature measurements. At room temperature, the simulations reveal thermal resonance shifts of 62.8 pm/K for silicon, 30.4 pm/K for gallium nitride, 16.8 pm/K for diamond. As a result of the lower thermo-optic coefficient the diamond resonator has a smaller temperature sensitivity. The studies on self-heating have shown, however, that it is superior to silicon at the extreme circulating power at resonance within the ring because owing to the high bandgap and high thermal conductivity of diamond the self-heating induced by two-photon absorption can be neglected.



Intensity distribution in a silicon microring resonator with bus waveguide at resonance.

Light-Matter Interactions on the 10nm Scale – from Quantum Fields to Mechanical Forces

C. Henkel [1], F. Stete [1], W. Koopman [1], M. Bargheer [1], G. Kewes [2], O. Benson [2], J. Jelken [1], S. Santer [1]

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We report on the modelling of light fields for experiments performed in Potsdam: extinction spectroscopy of core-shell gold nano-particles with J-aggregates as absorbers and polarised light diffraction from a polymer film doped with azo-benzene chromophores that develops gratings under holographic irradiation.

Core-Shell Nanoparticles as Plasmonic Resonators

The group of M. Bargheer works with aqueous solutions of gold nano-rods covered with a thin shell of the cyanine dye TDBC that forms J-aggregates [**?**]. The standard modelling with Mie-Gans theory for elliptic particles [1] predicts a 'shell mode' that coincides in frequency with the resonance of the J-aggregates. We explain why this mode is not observed in measurements of the extinction spectrum: the nano-rod is a resonator with a mode volume so small that even a one-plasmon excitation saturates the narrow transition of the absorber shell. Including the saturation effect due to the one-plasmon field yields excellent agreement with experiment for different sizes of nano-rods. This highlights the challenge of modelling quantum electrodynamics in nano-structures with highly polarisable emitters [2, 3].

Photomechanical Deformation of Azo-Benzene-doped Polymer Films

The group of S. Santer studies thin films that are irradiated with a holographic light pattern (polarisation-controlled two-beam interference). The light drives the *trans-cis* isomerisation of azo-benzene in both directions. One observes a bulk birefringence grating by diffracting a probe beam and the growth of a surface relief grating by taking simultaneously AFM scans [4]. The data are fitted with a combination of Raman-Nath thin grating theory and continuum mechanics for the photo-induced alignment of the polymer material. The goal is to clarify the origin of mechanical stresses (above $100\,\mathrm{MPa}$) that must be at work in these glassy, hard materials [5, 6].

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FE Simulation of a Dipole Emitter Coupled to an Inverted Diamond Nanocone

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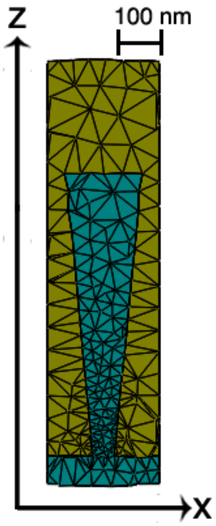
Unleashing the potential of quantum technologies requires efficient extraction of single photons from emitters. Here, we propose an inverted diamond nanocone structure for the efficient fibre coupling of single emitter fluorescence. We simulate far-field intensities and determine fibre coupling efficiencies of up to 86%.



An example inverted diamond nanocone

Motivation

Single, optically active quantum systems, such as single photon sources and quantum memories are important building blocks for quantum technologies. In order to achieve sensitive quantum sensors or high-rate quantum communication devices, efficient optical coupling to such quantum systems is required. Due to the high refractive index of host materials, coupling light in and out of the quantum systems across the material–air interface constitutes a fundamental challenge.

Proposed Design and Simulation Method

In this work, we focus on a device that is simple in design and easy to fabricate but still enables photon extraction efficiencies as high as in more complex designs. In particular, we optimize numerically the coupling efficiency of a dipole emitter inside an inverted diamond nanocone to a single mode optical fibre. Diamond nanocone structures can be fabricated by angled etching techniques [1].

We use JCMsuite, a finite element based software, to simulate far-field field and intensity distributions. By calculating the overlap integral between this far-field distribution and a fundamental Gaussian fibre mode, we determine a theoretical upper limit of the dipole-to-fibre coupling efficiency.

Results

From our simulations, we determine a parameter set that defines the nanostructure such that a dipole to fibre mode coupling efficiency of up to 86% can be extracted. By introducing additional constraints derived from realistic limitations in nanofabrication, we find coupling efficiencies of up to 84%.

Acknowledgements

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Modeling Landau Damping in Atom-Surface Quantum Friction

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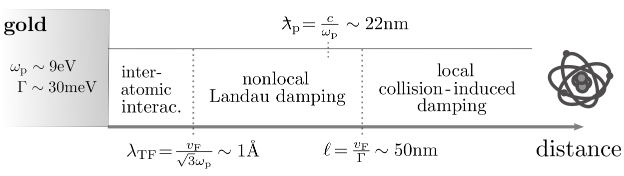
We discuss the impact of spatial dispersion on atom-surface quantum friction. Comparing different models for the material's electromagnetic response, we assess their validity as well as their predictive power and highlight the importance of incorporating Landau damping in the description.

Quantum friction is significantly enhanced due to Landau damping

Spatial dispersion becomes an important feature in the electromagnetic response of conductors, as soon as the dominating wavelength is of the order of or smaller than the mean free path of the electrons in the material. In this case, the phase velocity of the electromagnetic wave matches or is smaller than the electron speed enabling a coherent interaction. The process is accompanied by a net energy transfer from the wave to the material, the so-called Landau damping.

In the context of atom-surface interactions, the relevant wavelengths are given by the distance between atom and surface. Especially in nonequilibrium situations, where non-contact frictional forces occur [1], such interactions substantially depend on the dissipative properties of the body. In this context, including the often neglected Landau damping was shown to increase friction by several orders of magnitude [2]. The estimate was based on the Boltzmann-Mermin model that is derived from fundamental principles, but comes to the price of high technical complexity.

In the present work, we contrast such results using both the standard and an extended version of the hydrodynamic model for the electromagnetic response of the material. We show that the standard hydrodynamic description is inadequate for evaluating the frictional force, since it completely neglects Landau damping. The extended version qualitatively resolves this issue. The main advantage is that the simplicity of the extended hydrodynamic model allows for an easier analysis of the impact of nonlocality which we illustrate with an example involving a thin slab. Further, in view of the serious challenges related to a numerical implementation of spatially dispersive material models, our analysis delineates the limitations of the numerically more convenient hydrodynamic model [3].



Visualization of the dominant dissipative process underlying atom-surface interactions as a function of distance. We display a surface made from gold with plasma frequency ω_p, dissipation rate Γ, Fermi velocity v_F and mean free path ℓ.

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Reduction of multipole moments in subwavelength periodic dipolar chains

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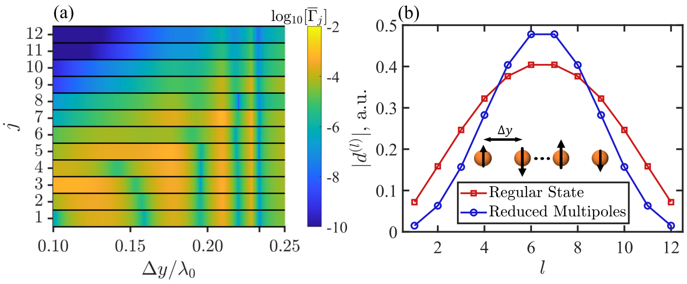
In this work we present a theoretical study of optical properties of a subwavelength linear periodic chain of dipolar scatterers. We show that very low emission rate of the band-edge modes in this system is related to the reduction of multipole contribtuions to it. We also show that the corresponding eigenmode has a peculiar resonator-like profile.

One-dimensional systems like periodic chains of scatterers have been appealing objects for a research not only from a fundamental side, but also as a waveguiding structure able to transmit signals with application in photonics, and plasmonics.

It was previously known that guided eigenmodes at the band-edge of such chains demonstrate a qubic growth of the quality factor with the number of scatterers $Q \sim N^3$ [1]. However, as we have shown in our recent work, when the system period is properly chosen, one can obtain a much more rapid growth of up to $\sim N^{6.8}$ for transverse modes [2]. In the presented work we elaborate on this from a point of view of multipole analysis, and find that such a behavior is a result of the simultaneous reduction of multipole contributions to the total emission rate up to some high multipole order j see Fig. (a).

Regular band-edge states (ones with $Q \sim N^3$) can be well described by a well known solution to a Tight-Binding (TB) model, $|\mathbf{d}_l| \sim \sin\left(\frac{\pi N l}{N+1}\right)$ with $\mathbf{d}_l$ being the dipole moment of the l^{th} particle. We found that when multipole reduction is observed, the state behaves quite differently (see Fig. b), and empirically found that it has a form of $|\mathbf{d}_l| \sim c_N \sin\left(\frac{\pi N l}{N+1}\right) + c_{N-2} \sin\left(\frac{\pi(N-2)l}{N+1}\right)$, where c_N, c_{N-2} - constants of opposite signs. The latter points to the presense of destructive interference between the two contributions, while an overall state looks like a cavity mode with substantially smaller dipole moment amplitudes at the edges, a situation known as Degenerate Band Edge (DBE) [3].

We believe that these findings are of importance for the field of photonics in general, and for the areas of research related to waveguiding one-dimensionan structures, in particular.



(a) Multipolar contributions of the emission rate $\overline{\Gamma}_j$ versus period $\Delta y/\lambda_0$. The chain consists of $N = 12$ particles. Note an additional tick on the x-axis specifying the point of multipole reduction (b) Regular band-edge mode profile (red), and a mode with reduced multipoles (blue).

Acknowledgements
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Micro-hole Collapsing Attributes in Microstructured Optical Fiber

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Over the last decade, a lot of attention has been administrated at microstructured optical fibers (MOFs), facilitated by their constitutional waveguiding attributes and the potential applications. We aim to explore the practical utility of micro-hole collapsing in MOFs, such as low-loss splicing between an MOF and standard fiber by employing an alternative analytical enhanced field model [1].

Summary

Optical fibers have become an indispensable component in modern telecommunications, and the standard step-index single-mode fibers (SMFs) have contributed an invincible global information highway. Presently, much of the research has relocated towards the enhancement of optical fiber based components and devices, taking superiority of novel speciality fibers such as microstructured optical fibers (MOFs) [2]. We can utilise deliberately collapsing of air-holes [3] as an additional dimension to MOFs, e.g., as a potential premise for evanescent field sensing applications in context to MOF-based photonic wires [4]. Also, the technique has been harnessed to produce Gaussian-like mode-field profile in multi-core MOFs [5]. In spite of that, low-loss splicing of MOF with an SMF can be achieved by collapsing the holes of MOF in a controlled manner [4], facilitating to mode-field expansion at the interface for accessing optimum coupling. We investigated the optical characteristics of the mode-field expansion (which can be quantified in terms of mode-field diameter (MFD)) for an MOF by utilizing an elegant technique based on controlled micro-hole collapse [3]. Enlargement of the mode-field profile for an MOF can be carried out by shrinking the diameter of air-holes through heat as localized heating allows surface tension of silica to collapse the air-holes. Relation between the diameter of holes d_0 and pitch Λ_0 (before collapse), and diameter of holes d and pitch Λ (after collapse) is quantified as [5]: $\Lambda^2 = \left(\Lambda_0^2 + \pi\sqrt{3}/6\left(d^2 - d_0^2\right)\right)$. We evaluated Petermann-1 MFD (increasing monotonically) against collapse ratio (see Fig. 1) by utilizing an enhanced field model, associated with trial field consisting of A, α, α_1, σ, B, α_2, and η as the field variables [1]: $E_t\left(r,\varphi\right) = e^{-\alpha r^2} - Ae^{-\alpha_1(\mathbf{r}-\sigma\Lambda)^2} \times (1+\mathbf{cos}\,6\varphi) - Be^{-\alpha_2(\mathbf{r}-\eta\Lambda\sqrt{3})^2} \times (1-\mathbf{cos}\,6\varphi)$; where Λ is the pitch. Inset of Fig. 1 illustrates the near-field at collapse ratio of 60%. We included the results based on Beam propagation method [3] for probing the correctness of our theoretical results. Coherent agreement between the results is accomplished. Further work is in progress.

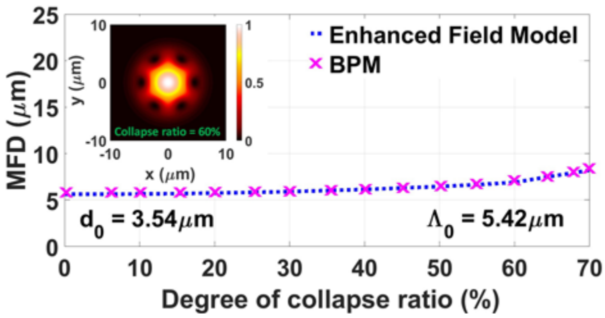

Fig. 1. *MFD against collapse ratio at 1.55μm.*

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Highly-sensitive laser focus positioning method with sub-micrometre accuracy using coherent Fourier scatterometry

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We report a novel method of focus determination with high sensitivity and submicrometre accuracy. The technique relies on the asymmetry in scattered far field from a nanosphere located at the surface of interest. The out-of-focus displacement of the probing beam manifests itself in unbalance of the signal of the differential detector located at the far field. Up-down scanning of the focussed field renders the error s-curve with a linear region that is slightly bigger than the corresponding vectorial Rayleigh range. We experimentally show that the focus can be determined not only for the surface with high optical contrast, such as silicon wafer but also for weakly reflecting surface, such as fused silica glass.

Further, for the probing wavelength of 405 nm, three sizes of the polystyrene latex (PSL) spheres, namely 200, 100, and 50 nm in diameter are tested. Higher sensitivity was obtained as the sphere diameter got smaller. However, due to the fact that the scattering cross-section decreases as the sixth power of the nanosphere diameter, we envision that further size reduction of the studied sphere will not contribute to a drastic improvement in sensitivity. We believe that the proposed method can find applications in bio/nano detection, micromachining, optical disk applications.

Design of light scattering nanoparticles for improved photon management in light-emitting devices

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Light-emitting devices based on organic electroluminescent or on quantum dot (QD) conversion layers face the challenge of a poor light extraction efficiency and in the latter case, of a limited absorption of the UV/blue excitation light by the QDs. We show that composite materials, exploiting the light scattering properties of nanoparticles, can efficiently improve these optical shortcomings. Here we provide guidelines for the design of such materials and discuss the range of applicability of the T-Matrix method used for that purpose.

QD-based light emitting diodes (LEDs) have gained increasing attention for display applications, that demand high color rendering, sharp contrast and energy efficiency. The narrow emission spectra of QDs, combined with their feasibility of solution deposition and patterning [1], provide QDs with a severe advantage over the established phosphor based light conversion. While their internal light conversion efficiencies approach unity [2], light management has to overcome optical shortcomings to facilitate a commercial success of QD displays. One of the key challenges is the combination of an efficient absorption of excitation light with a directional out-coupling of QDs down-converted emission. While the absorption of excitation light is limited by the small scattering and absorption cross-section of QDs, the optimization of the out-coupling efficiency faces similar challenges as organic LEDs (OLEDs). However, in contrast to OLEDs, where a metallic rear reflector directs light towards the device front, an efficient in-coupling of excitation light needs to be preserved. For this purpose, a short-pass filter, commonly a distributed Bragg reflector (DBR), is required, which combines a high transmittance for the excitation source with a strong reflectance for the QD emission.

In this communication, we first summarize the superposition T-matrix scheme to model light scattering by large disordered nanoparticle ensembles in layered media [3].

We demonstrate, that light scattering composite layers can be inserted in thin-film OLED stacks to improve their out-coupling efficiency.

Next, we investigate the potential of scattering as a light management tool in optically thick QD conversion layers. To this end, we introduce the concept of a particle-based, wavelength selective reflector. Here we cover optimization of the scattering characteristics of single core-shell nanoparticles and analyze the collective optical response of particle ensembles of more than 24000 individual scatterers, performed with SMUTHI [4], an in-house developed Python package. Finally, we report a four times increased absorption of UV-light, combined with a twofold out-coupling efficiency in the desired forward direction, with respect to a DBR-based QD conversion layer. Our designs pave the way to light management films that can be realized with industrially relevant printing methods.

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Nonlinear Interaction of Femtosecond Pulses with Glassy Chalcogenides

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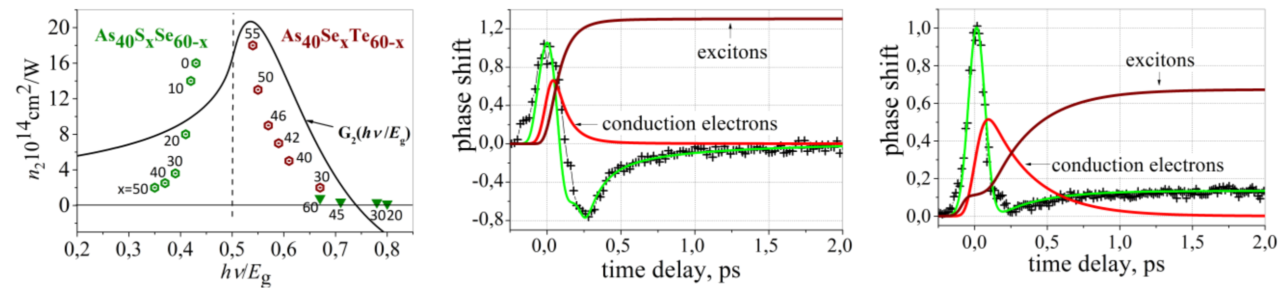
Femtosecond-scale nonlinear optical response of glassy chalcogenides of the systems As-S-Se and As-Se-Te at frequencies near their single- and two-photon bandgaps is studied in experiment and in a numerical model. The determining role of gap states in photosensitivity of the disordered chalcogenides is demonstrated.

We study the role of gap states in the nonlinear optical response of glassy chalcogenide semiconductors illuminated by femtosecond (fs) laser pulses by comparative analysis of the results of numerical modeling and measurements by using two pump-probe method realizations [1,2]. These disordered materials exhibit high photosensitivity when illuminated at frequencies near their single- and two-photon bandgaps. By use of several glass compositions with bandgap energy E_g in the range of 1.8-2.4 eV (As-S-Se) and of 1.1-1.4 eV (As-Se-Te) illuminated by fs pulses with peak wavelength λ of 790 nm or 1570 nm, the ratio of the photon energy $h\nu$ to E_g was tailored from 0.35 to 0.8. Magnitudes of the nonlinear refractive index n_2 have been evaluated as described in [1,2], plotted as functions of $h\nu/E_g$ and compared with the spectral function $G_2(h\nu/E_g)$ of n_2 known from the theory of non-linear optical response of direct-gap crystalline semiconductors (Fig.1a). Femtosecond-scale variation of dielectric constant ε due to the third-order optical nonlinearity and charge carriers kinetics (the phase shift in Fig.1b,c is proportional to ε) is driven by the single- or two-photon transitions to the gap states depending on $h\nu/E_g$. Tailoring of $h\nu/E_g$ allows managing long-time scale variation of ε that is important for development of the technology of chalcogenide glass processing by fs lasers.



a) b) c)

Figure 1. Magnitudes of n_2 evaluated at λ = 790 nm (triangles) and 1570 nm (hexagons) (a). Phase shift of the probe pulse depending on its time delay respectively to the pump pulse with the peak intensity of 900 GW/cm^2 (b) and 80 GW/cm^2 (c) at λ = 790 nm in the samples: $As_{40}S_{60}$ (b) and $As_{40}S_{15}Se_{45}$ (c), the phase shift measured (symbols) and calculated (green lines). Densities of excitons and conduction electrons (red lines) are multiplied to $10/N_c$ (b) and $10^4/N_c$ (c), N_c is the critical plasma density.

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Calculating Complex-Frequency Eigenmodes of Long-Period Photonic Crystal Slabs Using Aperiodic Fourier Modal Method

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We present an iterative numerical method for calculating eigenmodes of photonic structures with 1D-periodicity, which is based on the aperiodic Fourier modal method. We demonstrate that the method is efficient for studying resonant properties of long-period diffractive structures (photonic crystal slabs and diffraction gratings) with periods up to at least 500λ. The proposed method is promising for the investigation of periodic photonic structures with defects and of quasiperiodic and random structures within the super-cell approach.

Numerical method

In the last decades, investigation of resonant optical properties of nanophotonic structures has attracted considerable attention [1, 2]. This is not only due to fundamental interest, but also due to the potential applications of resonant structures for spectral and spatial filtering, lasing and sensing, to name a few. Resonant optical effects in photonic structures are associated with the excitation of leaky eigenmodes. It has been shown that the knowledge of the eigenmodes enables fast and accurate prediction of the optical properties of the structure under varying excitation conditions [3, 4, 5]. Thus, the ability to rigorously calculate the eigenmodes of nanophotonic structures is of crucial importance.

In this work, we present an iterative method that is based on the aperiodic Fourier modal method and enables calculating complex frequencies and field distributions of quasiguided modes of photonic crystal slabs with one-dimensional periodicity [6]. The method employs the rotation of the investigated periodic structure by 90 degrees and artificial periodization of the obtained rotated structure (i.e. the periodization in the direction perpendicular to the initial periodicity direction). The adjacent periods of the obtained structure are optically isolated using perfectly matched layers. The eigenfrequencies of the initial structure are found from a generalized eigenvalue problem involving the scattering matrix of the rotated structure and are iteratively refined. We demonstrate that the method is particularly useful for investigating long-period diffraction gratings and photonic crystal slabs. Possible applications include investigating the impact of defects on resonant properties of photonic crystal slabs and studying optical properties of random and quasiperiodic photonic structures. With an increase in the period of such a structure, the number of the eigenmodes increases as well. To distinguish between these modes, one needs to analyze its field distributions.

Acknowledgments

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Surface roughness in finite element meshes

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We present a practical approach for constructing finite element meshes with given autocorrelation function and show example applications in nanophotonics using the discontinuous Galerkin time domain method.

Surface roughness plays an important role in physical and chemical phenomena and is therefore of great importance in science and engineering. In the broad area of nanophotonics it is known that the optical responses in general can be significantly changed by surface roughness, which, for example, plays a role in the light scattering by small particles, influences the optical properties of plasmonic nanostructures, leads to losses in photonic crystal waveguides, changes the performance of hyperbolic metamaterials, affects the Casimir force and enables surface-enhanced Raman spectroscopy. Surface roughness is the deviation in normal direction of a real surface from its nominal form and is typically characterized by the root mean squared (rms) roughness R_q and the correlation length l. A mesh with given rms roughness can be easily achieved by simply moving points on the mesh of the nominal surface in the normal direction by an amount set by uncorrelated random numbers. In order to introduce a finite correlation length, one option is to perform a convolution of the uncorrelated random numbers with a filter function of the desired form [1]. This method, which is known as the spectral method, is suitable for regular grids of rectangular surfaces.

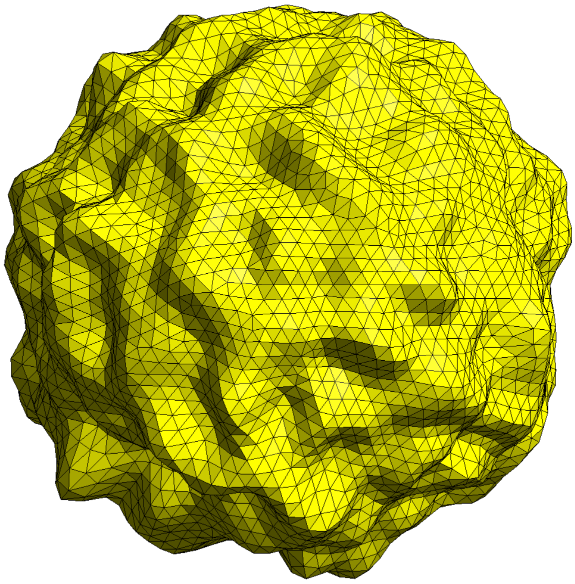

Fig. 1. Unstructured mesh of a rough sphere with radius r, rms roughness $R_\mathrm{q} = 0.05$, correlation length $l/r = 0.15$ and element size $h/r = 0.05$.

As an alternative to the spectral method, we discuss how one can instead work directly with unstructured meshes of the nominal structure and create correlated random numbers by use of a well-known method based on decomposition of of the autocorrelation matrix [2]. This approach is suitable for general surfaces such as a sphere which is shown in fig. 1.

The resulting meshes can be used for finite element methods in nanophotonics but also in various other fields in science and engineering.

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Contour integral methods for computing nanophotonic resonances

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We review algorithms for the solution of nonlinear eigenvalue problems resulting from Maxwell's equations. Numerical realizations of the algorithms are applied to compute resonances in nanophotonic systems with material dispersion.

Contour integrals methods [1, 2, 3, 4] can be used to solve nonlinear eigenvalue problems [5]. An approximate subspace is constructed corresponding to specific eigenvectors whose eigenvalues are located inside a chosen region in the complex plane. In nanophotonics, the material dispersion causes the nonlinearity of the occurring eigenproblems and is often described by the Drude-Lorentz model or rational fits to measured material data [6, 7].

In this contribution, we review contour integral algorithms and demonstrate a numerical implementation for computing nanophotonic resonances beyond the Drude-Lorentz model [8]. We apply a finite element based implementation of the algorithm proposed by Beyn [2] to compute resonances based on the hydrodynamic Drude model. The resonances are then used to perform a modal analysis of the extinction cross section. The implementation essentially relies on solving the time-harmonic Maxwell's equations in the frequency domain. The numerical realization is straightforward as standard scattering solvers can be used for the contour integration and no auxiliary fields have to be introduced for implementing the dispersion models.

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Numerical realization of the Riesz projection expansion

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The Riesz projection method [1] and a numerical realization is presented. The approach is applied to expand quantities which are linear or quadratic in the electric field. Furthermore, numerical properties of the method are studied.

Highly specialized Maxwell's equation solvers allow for an efficient evaluation of scattering problems, such as the interaction between light sources and leaky nano-optical resonators. To gain physical insights, modal expansions are a common approach [2]. In this way, the effect of intrinsic properties of the resonator on desired optical properties of the whole system can be investigated. This provides the basis for the design of optimized devices. As energy dissipation leads to non-Hermitian operators, the evaluation of expansion coefficients becomes a challenging task. The recently proposed contour integral method based on Riesz projections [1] exploits the power of state of the art algorithms for solving arbitrary scattering problems in order to evaluate expansion coefficients for resonance expansions.

In this contribution, a numerical realization of the Riesz projection method is presented which exploits symmetry properties and the possibility of parallelization. It is applied to expand the Purcell factor in two different ways as well as the energy of the electric field. The expansion of quadratic forms is based on separate analytic continuations of the electric field and its complex conjugate [3]. Furthermore, numerical properties of the method are studied.

We acknowledge funding by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy The Berlin Mathematics Research Center MATH+ (EXC-2046/1, project ID: 390685689). We further acknowledge support by the Helmholtz Excellence Cluster SolarMath.

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The Shape Derivative for Uncertainty Quantification and Optimization of Perfectly Electric Conducting Gratings

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This work explores the use of the shape derivative as a tool in computational electromagnetics for quantifying the effects of surface random perturbations as well as for optimizing the geometry of perfect electric conducting gratings.

Introduction

Gratings are periodic structures used in several applications such as spectroscopy, energy conversion, beam splitters, and so on. For this reason, it is mandatory to have reliable, robust, and accurate numerical tools able to model gratings while retaining reasonable computational times. Over the last years, significant work on so-called *shape derivatives* has opened a path to build and perform such simulations. In general terms, the shape derivative of a given field u over a nominal shape is defined as the limit $\lim_{\varepsilon\to 0}(u^\varepsilon - u)/\varepsilon$ where the field u^ε is computed over a family of perturbed shapes indicated by the superscript ε. In this work, we show how shape derivatives quantify the impact of small random perturbations and optimize the geometry with respect to a certain functionals. Moreover, the diffracted field is obtained by solving the electric field integral equation for perfectly electric conducting gratings and the implementation of the boundary element method.

Quantification of surface random perturbations

An algorithm that is able to quantify the impact surface random perturbations on the grating diffraction efficiency is proposed and compared to the Monte Carlo method [1]. The proposed algorithm consists of a sparse approximation and the use of a deterministic approach based on the shape derivative to compute statistical moments (mean and variance). This method reduces the computational time from hours (Monte Carlo approach) to minutes without significant cost in the accuracy (< 1 %).

Profile optimization

We also explores the implementation of first- and second-order optimization algorithms [2] that optimize the grating geometry to maximize the diffraction efficiency or to reach a particular given one. The second-order approach converges faster than the first-order one and outperforms it when the solution gets closer to a local maximum (minimum). The second-order method computational efficiency is further improved by conveniently calculating the involved Hessian every M iterations. These algorithms are especially efficient when the number of parameters that describe the geometry becomes large.

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An aperiodic differential method associated with the FFF: a numerical tool for integrated optic waveguide modelization

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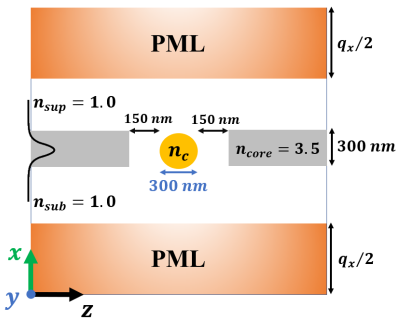
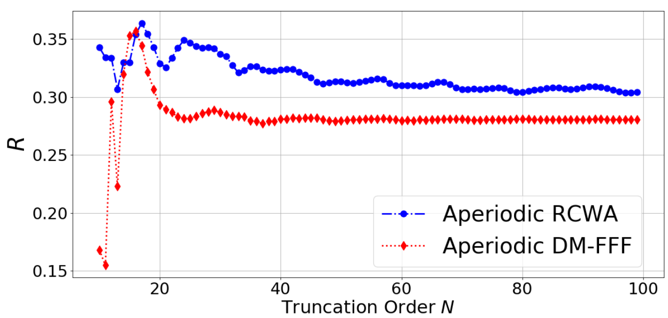
The differential method (DM) associated with Fast Fourier Factorization (FFF) has demonstrated its effectiveness with the modeling of metallic periodic diffractive structure especially when the grating is illuminated with TM polarization. In this paper, we will exploit for the first time the use of the DM-FFF in the guided optics domain and how this method can be a powerful solution for the design of complex shaped photonic devices.

Numerical validation and comparison

The DM-FFF [1] is known for diffraction grating modelization. Hugonin et al. [2] have demonstrated that performing a complex coordinate transformation to the formulation of Maxwell's equations can play the role of perfectly matched layers (PMLs). Thus, the classical RCWA will turn into an aperiodic method (a-RCWA) used for the modeling of dielectric waveguides structures. Following a similar approach, an implementation of PMLs with the DM-FFF has been introduced. The geometry of Fig.1 is now considered. The waveguide is excited from the left with its first guided mode in TM polarization (H_y, E_x and E_z) with $\lambda = 975nm$. As it is expected, the a-RCWA converge slowly due to the staircase approximation [3]. On the other hand, the a-DM-FFF demonstrate its fast convergence beyond $N = 30$ harmonics remaining stable along the evolution of N. Indeed, in this case the electric field boundary conditions are respected on the periphery of the cylinder.



(a)



(b)

Fig. 1.: (a) Integrated optic structure with $n_c = 1.0 + j4.0$. PMLs of thickness q_x are surrounding the structure b) Evolution of the reflection coefficient R w.r.t N using the a-RCWA and a-DM-FFF

This work shows, for the first time, the effectiveness of the a-DM-FFF with guided structures. We believe that this method will open the way for researchers and engineers to simulate and model new arbitrary shaped guided structure that was considered as problematic before.

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Multi-resonant plasmonic supercells

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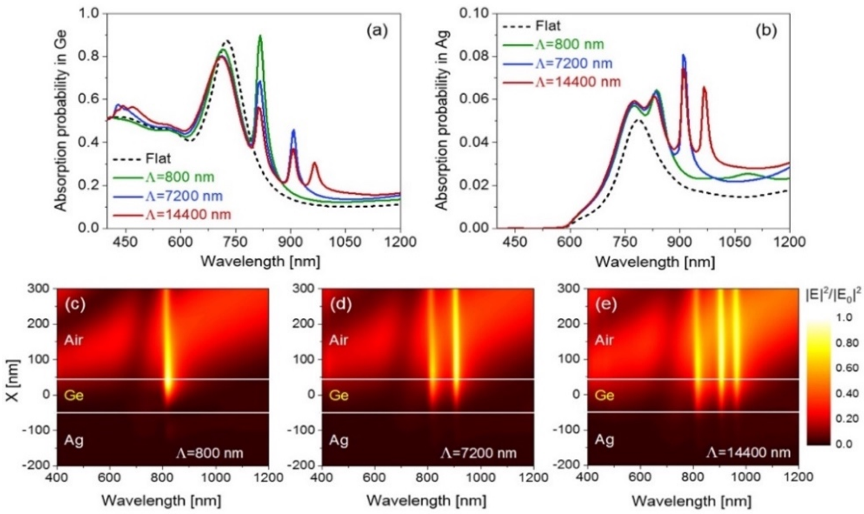
Multiple diffractive surface modulations can concurrently couple the light to several electromagnetic surface waves [1]. We presented a novel semiconductor-based plasmonic multi-resonant supercell structure with a broad range of applicability in harvesting the light over an extensive wavelength range and angles of incidence [2]. The plasmonic multi-resonant bands were realized by incorporation of several encoded periods in a conventional diffraction grating structure, ensuring that the properties of a single periodic structure in excitation wavelengths and angular dependency were preserved by the supported supercell structure. As it is shown in the figure, the concept for three encoded periods corresponding to different spatial frequencies of surface modulation function at a silver:germanium interface shows a plasmon-enhanced absorption probability of 18.13% in a wide wavelength band of 400-1200 nm. This translates to an enhanced absorption factor of 7.5% in the Ge photoactive layer for a multi-band structure compared to that of a single-band.



Absorption probability in (a) Ag, and (b) Ge layers for different periods. The dash lines show the absorption of flat structures. (c) Normalized electric field intensity corresponding to gratings with Λ=800 nm, (d) Λ=7200 nm, and (e) Λ=14400 nm within their layer configuration.

This work is based on both realistic theoretical and experimental data to show the modal interferences in multi-diffractive gratings [2-3], and how a plasmon-mediated absorption band extends over a wide wavelength window upon the surface development. In addition, the using of this diffractive platform in highly integrated and compact lab-on-chip biosystems will be discussed.

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Absolute refractive index dispersion determination from angle-resolved photonic crystal slab transmission spectra

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Photonic crystal slabs show guided-mode resonances in transmission measurements. The resonance wavelengths depend on the materials' refractive indices and the angle of incidence. We propose to obtain the in-plain refractive index dispersion of a material by deposition on a grating structure and fitting the angle-resolved transmission spectra with the Bragg equation.

Knowing the material properties is a key factor for correct simulations of real-world devices. In the field of organic optoelectronics, new materials are used to achieve high device performances. Organic materials are often anisotropic. It is therefore necessary to measure the in-plane refractive index of these materials. We propose the use of a one-dimensional photonic crystal slab (Fig. (a)) for in-plane refractive index determination and to obtain the full refractive index dispersion from photo-goniometric angle-resolved measurements of the guided mode resonance (Fig. (b)).

Here, the resonance position is calculated from the Bragg equation $\lambda_{\mathrm{res}} = \Lambda(n_{\mathrm{eff}} - \sin\vartheta)$, where Λ is the grating's period and ϑ the illumination angle (Fig. (c)). For shallow gratings, the effective index n_{eff} of the resonant mode is calculated approximately from the transfer-matrix analysis [1] of the corresponding unstructured slab waveguide [2]. The unknown refractive index is used as a fitting parameter in the transfer-matrix method to obtain the measured pair $(\lambda_{\mathrm{res}}, \vartheta)$. In contrast to conventional ellipsometry, the desired refractive index is directly used as the fitting parameter.

We validate our approach using the finite-difference time-domain (FDTD) method, compare the direct transmission and the orthogonal polarizer setup [3], perform an error analysis, and present measurement examples.

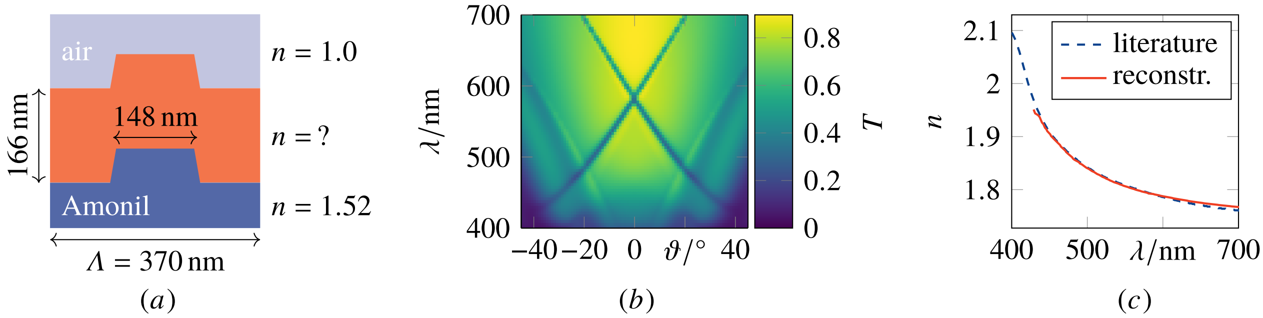

Figure. *Numeric validation of proposed method. (a) Material under test (red) on photoresist (Amonil) nanostructure. (b) FDTD-simulated angle-resolved transmission spectrum for OLED material NPB. (c) Refractive index of NPB reconstructed from the guided-mode resonance positions in (b) and the Bragg equation, compared to the literature value used in the simulation.*

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Implications on Mode-Field Expansion in Microstructured Optical Fiber

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Abstract: We explore one of the potential application aspects of air-holes collapsing in hexagonal microstructured optical fiber (H-MOF) as mode-field expansion (MFE) which can be utilized for minimizing the splice losses between dissimilar fibers, by employing finite-element method (FEM) in combination with Ring Model [1].

Introduction

Microstructured optical fibers (MOFs) [2] exhibit distinctive characteristics in contrast to classical optical fibers possessed by their flexible geometry. Collapsing of air-holes have significant efficacy on optical performance of MOFs and can be utilized in multitude of potential applications such as polarization maintaining MOF-based interfereometric gyroscope, mode-converters, and the Mach-Zehnder interferometer based refractive index sensor [3-5]. Therefore, we intend to investigate the practical utility of mode-field expansion (MFE) furnished by collapsing of air-holes in high-index core H-MOF [6] by employing the FEM in conjunction with earlier developed Ring Model [1].

Results and conclusion

MOF-based MFE is effectuated by uniform shrinking of all air-holes through heating (keeping the collapse (or shrinkage) ratio constant), and the relation between the diameter of air-holes d_0, pitch Λ_0 (before collapsing), and the diameter of air-holes d, pitch Λ (after collapsing) can be quantified as [6]: $\Lambda^2 = \Lambda_0^2 + c_1\left(d^2 - d_0^2\right)$; where $c_1 = \pi/2\sqrt{3}$ is a constant, and the degree of collapse ratio is defined as: $\rho = \left(1 - d/d_0\right)$ with $0 \le \rho \le 1$. Mode-field expansion in H-MOF (with $d_0 = 3.54$ µm and $\Lambda_0 = 5.42$ µm) is explored by evaluating the mode-field diameter (MFD). Figure 1 illustrates MFD as a function of collapse ratio, increasing monotonically as collapse ratio is increased from $\rho = 0\%$ to 60%; as decrease in air-hole diameter facilitates the expansion of mode-field pattern into the porous cladding. Thus, one can tune the MFD by controlling the collapse ratio for the optimum mode-field matching (to reduce the losses) during coupling with other fibers (or waveguides). Inset (a) of Fig. 1 depicts the geometrical structure of H-MOF [1], used in our simulation, and inset (b) illustrates the generated near-field profile for $\rho = 30\%$ at 1.55µm. Further work is in progress.

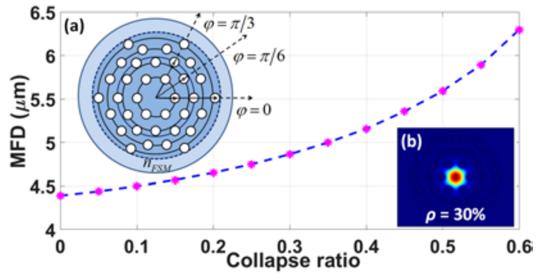

Fig.1. MFD against collapse ratio.

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Comparison of rigorous microscope simulations for metrological determination of bidirectional measurands

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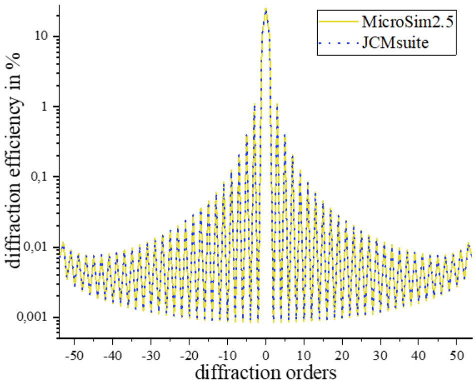
In this contribution, we evaluate the performances of two rigorous diffraction calculation methods with each other and with actual microscopic measurements. While the numerical calculated diffraction spectra agree perfectly with each other, there are significant differences in the image formation results.

Length measurements between two opposing edges of countering orientations are called bidirectional measurements. They include e.g. measurements of structure widths (in semiconductor industry also called critical dimensions) or diameters. In the field of optical microscopy, they require sophisticated model-based edge detection algorithms to achieve small measurement uncertainties [1]. The key feature of the edge detection algorithm is the rigorous simulation of the microscope imaging. The simulation is divided into two steps: at first, the diffraction spectrum of the incident light is determined by solving Maxwell's equations. In the second step the image reconstruction in the image plane is conducted by taking all the imaging parameters of the microscope into account. We apply Hopkins pupil approach, where the entrance pupil is discretized and for each pupil point the electrical and/or magnetic fields of all diffracted orders within the numerical aperture of the objective are summed up. The intensity distributions in the image plane is calculated using an FFT and for partly coherent illumination, corresponding to each pupil point summed up over all pupil points. The intensity levels in the edge profiles corresponding to the edge position are called threshold values. They are derived from the simulated images and can be applied to analyze measured image profiles in order to locate the measured edge positions and with it the measured structure width. The goal of this work is to evaluate the accuracy and correctness of the different simulation tools. Since all rigorous models apply specific approximations, which may introduce systematic deviations, simple convergency considerations are not sufficient for this purpose. At PTB, two rigorous modeling software packages MicroSim2.5 and the JCMsuite are applied. They rely on the fundamental algorithms of the rigorous coupled wave analysis (RCWA) and the finite element method (FEM), respectively [2,3]. We compare the simulation results of the two rigorous methods with each other for the example of imaging of binary line gratings in a high NA UV- transmission microscope. The dimensions of the different gratings are adapted from a test suite which was developed by NIST for such comparisons [4]. First results indicate a high agreement in the calculated diffraction spectra between the two solvers. However, the calculated image profiles deviate from each other significantly. To offer more insight, the results of this work are compared with the results of a prior comparison [4] and occurring deviations are discussed.



Comparison of the diffraction efficiencies of MicroSim2.5 and JCMsuite

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Shallow Nano-Textures for Light Management in Solution-Processed Perovskite Solar Cells

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Abstract:

In just about a decade of research metal halide perovskites have led to highly efficient thin film solar cells and a suitable tandem solar cell partner for established silicon photovoltaics. Further increase of power conversion efficiencies is expected to be achieved with adequate light management. However, spin-coating of perovskite films – currently the dominant technology for perovskite solar cells – is not compatible with standard pyramidal light trapping textures in silicon photovoltaics.

This work reports enhanced power conversion efficiencies thanks to light management in spin-coated metal halide perovskite single junction solar cells on shallow nano-textures.

We demonstrate a nano-textured solar cell based on triple cation perovskite with 19.6% power conversion efficiency and a relative efficiency increase of 3% with respect to its planar reference. For light management diverse textures (inverted pyramids, hexagonal sinusoidal and pillar-like structures) were transferred onto glass substrates via UV nanoimprint lithography for spin-coated perovskite solar cell devices. Scanning electron microscopy images of spin-coated perovskite on the nano-textures show a steady wetting of the perovskite material and a smooth surface for further processing. External quantum efficiency and reflectance measurements on these devices display a magnified short circuit current density of about +1 mA cm^{-2} with respect to their planar reference cells. Optical simulations based on the finite element method allow to ascribe the enhanced current densities to nano-structure induced light in-coupling. For electronic optimization we compare different charge carrier selective contacts. Cell stability was examined with maximum power point tracking. The impact of nanostructures on short-circuit current density, open circuit voltage and fill-factor in the solar cell devices are discussed in detail.

The shallow nano-textures are promising candidates for advanced light management in perovskite-silicon tandem solar cells with solution-processed perovskite top cell and for overcoming current optical losses in devices with planar interfaces only.

The Role of Electromagnetic Scattering in the Formation of Laser-induced Periodic Surface Structures

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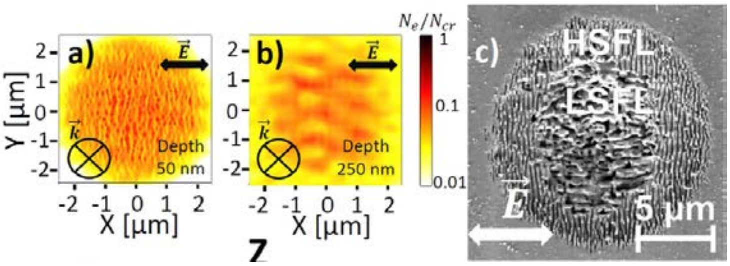
Laser-induced periodic surface structures (LIPSS) [1] are a universal phenomenon that is accompanying laser materials processing. These surface nanostructures pave a simple way for surface functionalization with numerous applications in optics, fluidics, tribology, medicine, etc. [1]. This contribution reviews the current view on the role of electromagnetic scattering in the formation of LIPSS.

Scattering and Interference as origin of LIPSS

In the ablative regime LIPSS emerge on almost any material (metals, semiconductors, and dielectrics) as a surface relief composed of periodic lines with periods close to or below the irradiation wavelength and with a clear correlation to the linear polarization of the radiation. During the last decade remarkable experimental and theoretical improvements in their formation mechanisms were obtained - all pointing toward ultrafast energy deposition mechanisms acting during the absorption of optical radiation that is scattered at the surface roughness and interfering with the laser beam [1-3].

The widely accepted analytical LIPSS-theory of J.E. Sipe et al. [4] was proven to almost quantitatively describe the absorption of laser radiation a rough surface of semiconductors [2]. This theory, however, remains restricted to the near-surface (selvedge) region and does not consider feedback mechanisms. Energy deposition to deeper lying sub-surface regions and multi-pulse effects must be approached numerically, e.g. by three-dimensional time-resolved *finite-difference time-domain* (FDTD) calculations. This was successfully demonstrated by Rudenko et al. [3] for the formation of LIPSS on fused silica surfaces upon fs-laser irradiation, see the example for laser-induced electrons in the following figure.



(a, b) Normalized laser-induced electron density distributions in silica calculated by 3D-FDTD for a 120 fs laser pulse (800 nm) at two different depths from the rough surface. (c) SEM micrograph of LIPSS on a quartz surface after irradiation with 20 laser pulses (150 fs, 800 nm, 5.8 J/cm^2) [3].

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Scanning Coherent Fourier Transformation Scatterometry – a New Model based Approach for Subresolution Metrology of Aperiodic Nano-Patterns

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Optical Scatterometry a.k.a. OCD is a well established metrology technique in semiconductor industry and beyond to optically measure nano-patterns down to 20 nm and below with visual light [1]. It is based on a rigorous modeling of the light diffracted by a grating sample. Unfortunately, it requires periodic patterns. Therefore, it cannot be measured directly in-die but on reference gratings located in the scribe line between the chips. Moreover, the light probe has to cover a certain number of periods resulting in metrology boxes of about 20 through 50 microns squared. With shrinking feature sizes, an increasing discrepancy is observed between the reference measurements and the real in-die patterns caused by the different location as well as by the different global shapes (periodic reference vs. non-periodic in-die features). Thus, there is a strong demand for real in-die measurements of aperiodic structures. Scanning Coherent Fourier Transformation Scatterometry could be a way to overcome this problem. In this paper, we present the basic principle of this method and provide some first numerical and experimental results. Furthermore, we present the theoretical model that is the core of this novel approach.

Basic Principle of SCFT

The basic principle of SCFT is shown in fig. 1. A laser beam is collimated and focused to the sample by means of an objective lens. A focus sensor (not shown here) keeps the surface of the sample in focus while scanning across. The focus spot is diffraction limited, i.e., ~1µm in diameter for red light. The reflected and diffracted light is then picked up by the same objective and directed via a beam splitter to either a detector array or a wave-front sensor (e.g. Shack Hartmann). Next, the measured wave-front is analyzed in terms of Zernike coefficients (NZK) and compared to a simulated set of NZK's. This is repeated until a sufficient match is obtained. Finally, the local pattern is retrieved from the simulation model.

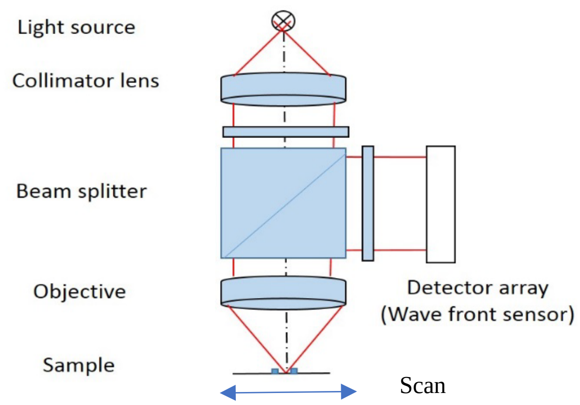

Figure 1: Basic principle of SCFT

Results

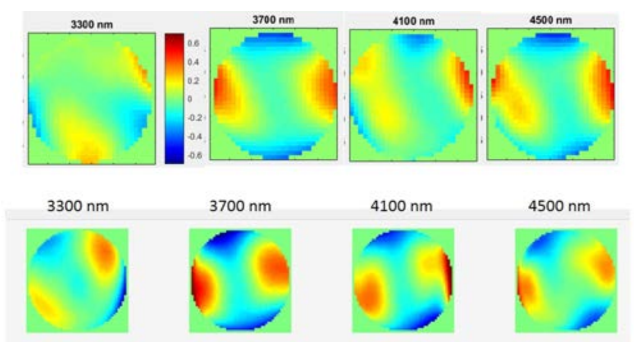

Fig.2: Simulated (bot.) vs. measured (top) wave-fronts

In order to prove the feasibility of the method a non-periodic pattern featuring lines and spaces 80 through 200 nm in width was written in Si by means of I-beam lithography. Some results are presented in fig. 2 comparing measurements and simulations when scanning across this pattern. The pictures demonstrate that SCFT is very position sensitive. In addition, the NZK analysis shows that even astigmatism and coma correlate very strong with the scan location whereas other aberrations do not. In conclusion, SCFT shows big potential for future metrology.

Resonant behavior of a single plasmonic helix

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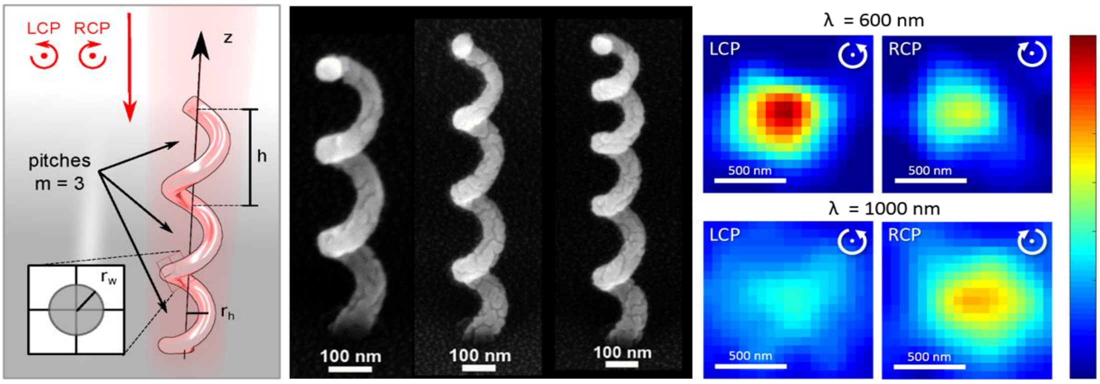
Abstract: We present an analytic model for the chiroptical response of helical nanostructures. Thereupon, a design tool for plasmonic helices being resonant in a desired spectral range was developed. Designed plasmonic helices were fabricated and investigated and shall be coupled to dipolar emitters in a next step.

Chiral plasmonic nanostructures will be of increasing importance for future applications in the field of nano-optics. To employ chiral geometries their linear resonant response in-line with the mechanism of efficient excitation has to be understood. Here, we investigate single plasmonic helices with strongly resonant features in the visible range. The helices are directly written with a focused electron beam [1,2] and conformally covered with silver after deposition [3]. Scanning confocal white-light spectroscopy is employed to measure extinction spectra of single nanostructures for left- and right-handed circular excitation. Based on simple geometric considerations the mechanism of excitation for either handedness is explained. This is formalized by an analytic model [4] that provides resonance conditions matching the results of full-field modeling. Based on the definition of an 'toggle' point, we derive design rules for the fabrication of helices being resonant in a desired wavelength range [5]. At the toggle point the net dipole moment of the helical antenna is vanishing what turns out to be especially well-suited for local dipole excitation. Thereby, local probes of chiral light [6] and even coupling to single quantum emitters may be realized. Corresponding work is under progress.



$$P^{\pm}_{\mathrm{ext},n} = \pm\frac{1}{4} mhE_0 j_{0,n} \{\mathrm{sinc}\,[mh(k \mp k_h - k_{\mathrm{FP}}] - \mathrm{sinc}\,[mh(k \mp k_h + k_{FP}]\}$$

Figure From left to right: Geometrical setting, scanning electron micrographs of silver coated helices, extinction maps of a helix with 4 turns. The analytical formula quantifies the excitation efficiencies for all types of resonances.

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Optimized designs for telecom-wavelength quantum light sources based on hybrid circular Bragg gratings

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We present FEM simulations of hybrid circular Bragg grating structures optimized for telecom O-band wavelengths. The designs exhibit near unity extraction efficiencies, high Purcell factors and single mode fiber compatibility, and are also robust to fabrication errors.

Quantum light sources emitting indistinguishable singe-photon or entangled photon states are key building blocks for future photonic quantum information technologies, such as quantum key distribution for secure communication. Especially quantum light sources based on epitaxial semiconductor quantum dots (QDs) are of particular interest, since they can be fabricated in a deterministic fashion, can cover a wide wavelength range and have the potential of scalability. Very recently, results on quantum light sources based on hybrid circular Bragg gratings (CBGs) with embedded QDs attracted much interest, since they achieved simultaneously high performances in all relevant (quantum) optical properties such as entanglement fidelity, single photon extraction efficiency and entangled-photon pair collection efficiency [1,2]. These results, however, where so far only limited to wavelengths below 900 nm, which are not compatible to optical fibers due to the high attenuation.

Here, we report on a design study for hybrid CBG devices operating at the telecom O-band [3]. We show optimized design parameters obtained from Finite Element simulations with Purcell factors of up to 30 and out-coupling efficiencies exceeding 95%, and investigate how these optical properties are affected by the structural parameters. We further show how these designs perform if fabrication deviations such as imperfectly etched grating walls are assumed. Additionally, the presented designs are robust towards deviation of the emitter's position within reported deterministic fabrication uncertainties. Finally we investigate the CBG-designs in terms of compatibility to optical single mode fibers and obtain up to 80% fiber coupling efficiency to off-the-shelf fibers without any further optimization.

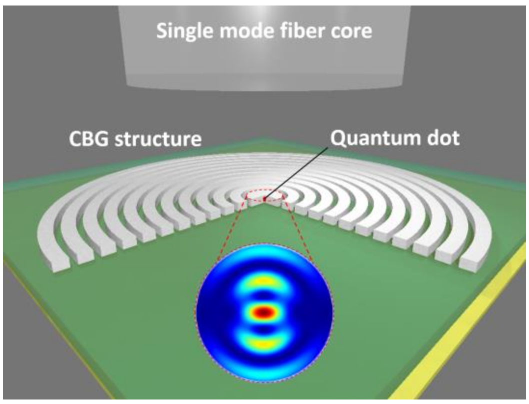

Fig. 1. Illustration of a hybrid CBG with an embedded QD, aligned to an optical single-mode fiber.

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Improving a micro-toroid's sensing limit through adding a thin dielectric shell

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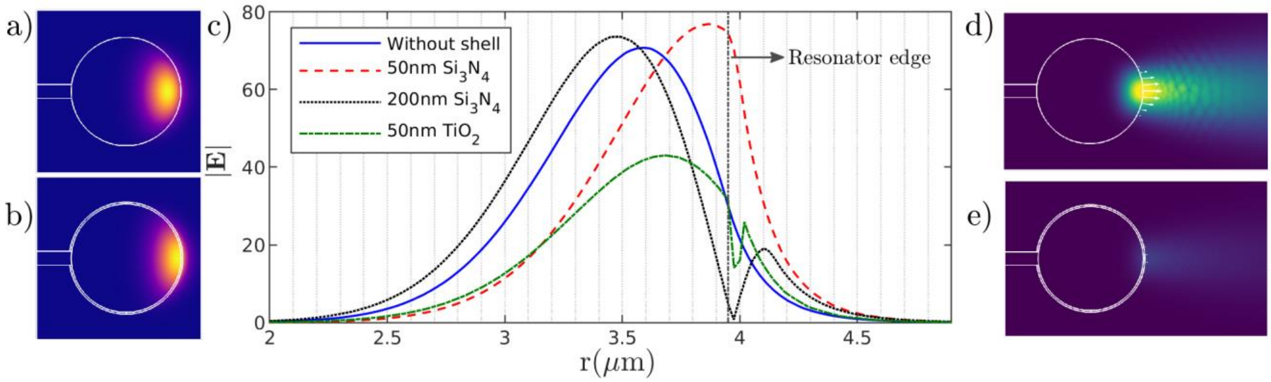
Abstract- Optical micro-resonators, capable of sustaining whispering gallery modes, have already proven their applicability as ultra-sensitive sensors [1], where the sensing limit is strongly dependent on the resonator's quality factor, the mode volume as well as on the electric field intensity at the sensing location. In the present work, we propose adding a thin dielectric shell with refractive index close to the micro-resonator's refractive index in order to improve the resonator's quality factor through reducing radiation loss. It is shown that adding a 50nm thick Si_3N_4 layer to the silica micro-toroid improves the quality factor by one order of magnitude through reducing the mode volume, while the electric field intensity at the sensing location is approximately doubled resulting in a significantly higher sensing limit.

Adding a thin, dielectric shell to the micro-toroid resonator to reduce the main loss contribution – namely the radiation loss - efficiently improves the resonator's quality factor and consequently the sensing limit. As the electric field strength at the sensing location is a determining quantity in the intended frequency shift, the shell should be designed in a manner that allows the evanescent tail of the electric field to penetrate to the ambient media. This requires a shell with a thickness in the range of the evanescent field's decay length and with a refractive index close to the one of the resonator. A silica micro-toroid (in air) with 8μm major and 1.5μm minor radius [2] is simulated using COMSOL Multiphysics, where the resonance frequency of the 93rd azimuthal mode occurs at 353.27THz with an associated mode volume of $60.7\mu m^3$. Two different dielectric shells using Si_3N_4 and TiO_2 have been added to the micro-toroid with thicknesses ranging from 50-200nm. Results show that the 50nm Si_3N_4 shell yields the highest quality factor as a consequence of both the decreased radiation loss (cf. Figure d, e) and the reduction of the mode volume to $53.3\ \mu m^3$, yielding a twofold electric field strength at the equator (cf. Figure a, b, c). As the resonance frequency shift is proportional to $|\boldsymbol{E}|^3$, the resulting frequency shift induced by the shell renders eight times larger and hence the sensing limit gets significantly improved.



Electric filed profile of the 93rd azimuthal mode in a micro-toroid a) without and, b) with a 50 nm Si_3N_4shell, and c) the electric field intensity on the equator for various shell thicknesses and compositions in comparison with the toroid without any shell. The radiation energy flux from a micro-toroid a) without and, b) with a 50 nm Si_3N_4shell.

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Small-scale online simulations in guided-wave photonics

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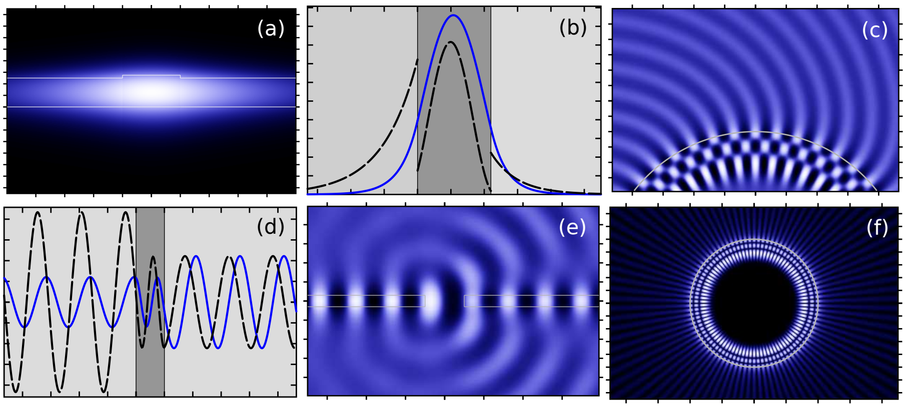
Nowadays, active web pages provide an ubiquitous computational platform. Even mobile devices are sufficiently powerful to facilitate locally physical simulations of moderate complexity. We discuss respective online solvers for a series of standard guided-wave eigenvalue- and scattering-problems in 1-D / 2-D.

Scientific simulations based on HTML5 / JavaScript

Current mobile devices provide a computing power that is comparable to the supercomputers of two decades ago. Hence, it should be possible to harness those facilities for highly advanced physical simulations, by the standards of 2000, even if things appear merely small-scale today. With HTML5 and JavaScript, recent years have seen some standardization in the encoding of web-pages and of active content, such that it now seems worthwhile to devote effort to the realization of projects for specialized scientific audiences. We illustrate this approach with a series of quasi-analytical solvers [1] for typical problems in guided wave photonics, as exemplified by the figure. The solvers are embedded in HTML5-pages, with a user-interface encoded in JavaScript, including graphics facilities (inline SVG). For the actual core computations, reasonably mature C++-sources exist. With a respective tool [2], these are *compiled* to JavaScript, and thus become directly available for the online computations. When comparing simulations carried out in a web-browser running the JavaScript code with a native program, where the respective C++-sources where compiled (gcc) and executed on the same desktop machine, we observed penalty factors < 3 in computational time.



Plots as generated by the online solvers [1] (annotations removed). (a) Mode of a rib waveguide with shallow etching, effective index approximation. (b) Guided TE- and TM-modes of a slab waveguide, Poynting vector. (c) Bend mode of second radial order supported by a curved dielectric interface, field snapshot. (d) Plane wave incidence on a dielectric slab, complex frequency-domain field. (e) Guided wave incidence at a hole in a slab waveguide, 2-D scattering problem, field snapshot. (f) Whispering-gallery resonance of a circular dielectric rod, interference of clockwise and anticlockwise propagating WGMs of second radial order, field modulus.

On the one hand, in a context of scientific simulations, this environment has certain shortcomings, mostly related to the particularities of the program language, and to security restrictions required for external web pages. On the other hand, all the burdens (compatibility, installation, distribution) that otherwise might prevent the use of an academic simulation tool by “others” are entirely absent. Our solvers have proven to be particularly useful for purposes of demonstration and teaching, but also for other tasks in integrated photonics design.

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From Nano-Optics to Quantum Mechanics: Method of Single Expression Extends its Domains

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The method of single expression established itself as a powerful alternative approach for solving multi-boundary problems in nano-optics. Applicability of the method for complex wave-matter interaction problems taking into account absorption, gain, high non-linearity and plasmonic effects was demonstrated many times. Current extension of the method shows its applicability for the problems in quantum mechanics.

Mathematical description of wave phenomena in nano-optics and quantum mechanics is similar and requires wavelength-scale analysis of wave propagation in nano-layers in optics and micro-particle interaction with potential barriers or wells for quantum mechanics. When dealing with problems in nano-optics and quantum mechanics the same fundamental approach of counter-propagating waves is often used and general solutions of the wave equations are presented as a sum of counter-propagating waves or a sum of exponentially increasing and decreasing amplitude distributions [1,2]. This approach relies on the superposition principle that is not always convenient as might lead to high complexity in multi-layer or multi-structure problems and can lead to significant errors or necessity of applying certain approximations when dealing with strong intensity-dependent non-linear wave-matter interaction problems. The non-traditional method of single expression (MSE) does not exploit the superposition principle, but rather uses resulting field representation and backward-propagation algorithm allowing to obtain correct steady-state solutions of boundary problems without approximations and at any value of wave intensity [3,4].

Successful application of the MSE for a wide range of wavelength-scale boundary problems in nano-optics served as a base for its extension to boundary problems in quantum mechanics as well. An isomorphism between the time-independent Schrödinger equation and the Helmholtz equation permits to present this extension of the MSE for quantum mechanics. Validation of the MSE for this new domain has been done for the problems of tunneling through rectangular potential barrier and resonant tunneling through double rectangular barriers. Within and outside of the barriers distributions of probability function and probability flow are easily obtained with the MSE. The results for reflection and transmission through barriers are in excellent agreement with the well known analytical solutions. This crucial validation step paves a way for the MSE to be widely used in the domain of quantum mechanics as well.

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Design of Octupolar nanopattern for Plasmonic sensing of Rotavirus

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In this work a two-dimensional Octupolar nanostructure made of gold nanopillars is designed by Finite Difference in Time Domain (FDTD) method, fabricated using Electron Beam Lithography (EBL) tool and used as Localized Surface Plasmonic Resonance (LSPR) based sensor for a specific and sensitive detection of low concentrations of Rotavirus.

Plasmonic nanostructures allow to engineer novel bio-sensing systems characterized by sensitive and specific responses [1]. In this work we design a two-dimensional gold nanostructure for a plasmonic sensing application. The nanopattern geometry we take into account is based on a periodic arrangement (fig.1a) of a unit cell (inset fig.1a) which gives rise to octupolar properties [2]. We performed numerical simulations based on FDTD method (fig. 1b) to study and to optimize the near-field and the plasmonic resonance of the pattern changing its characteristic sizes. Successively, we fabricated it using EBL tool. After functionalization with a specific antibody we tested our nanopattern as sensor based on the spectral frequency shift of the LSPR to detect low concentrations of Rotavirus. As widely reported in literature, LSPR sensors represent a good platform for developing highly efficient portable systems for a real-time, label-free and low cost bio-detection [3]. Testing various concentration of Rotavirus and other viruses (HBV1 and EVA), we demonstrate the possibility to detect in specific way amounts lower than 10^3 PFU/ml of the Rotavirus in water using a very low sample volume (2 µl). These results suggest that our device is promising to develop rapid, simple, very sensitive and specific immunoassay for biological analytes.

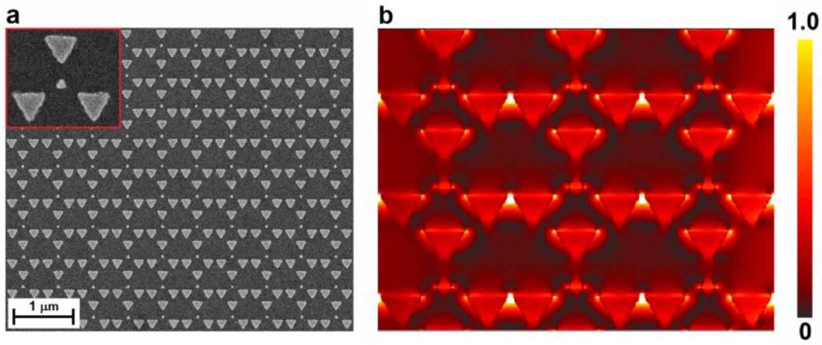

Fig.1: SEM image (a) and simulation of near-field distributions (b) of the octupolar nanopattern.

Acknowledgement

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Quasinormal Modes Expansion Techniques: Study of the Convergence Rate

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We study the convergence rate of quasinormal modes expansion techniques applied to the calculation of the cross-section of plasmonic nanoresonators. We test different formulations of the quasinormal modes expansion as well as different closed-form expressions for the expansion coefficients.

Photonic and plasmonic nanoresonators are dielectric or metallic optical devices that confine light at a scale smaller than the wavelength. They are used in various applications, such as high-performance sensors, light focusing below the diffraction limit, nanolasers, or solid-state single-photon sources.

With today's numerical tools, nanoresonators can be designed numerically by solving Maxwell's equations. However, such numerical studies need to repeat many independent computations, as the polarization, incidence, and frequency of the excitation fields are varied. The numerical load may be heavy, and, above all, the computed data obtained with these brute-force calculations may still hide much knowledge about the physical mechanisms at play. To bypass such difficulties, it is tempting to rely on mode theory, which represents the resonator response as a weighted sum of mode contributions [1]. In the case of dissipative optical resonators, the eigenmodes of the system are usually referred to as quasinormal modes (QNMs), or resonance states.

Modal expansion techniques rely on two crucial steps: the numerical computation of the modes (complex eigenfrequency and field distribution) [2] and the analytical calculation of their excitation coefficient, which is related to the weight of the mode in a modal expansion. Different closed-form expressions for the excitation coefficient can be derived from various theoretical frameworks [1,3-5]. Obviously, when considering a truncated modal expansion (i.e., for a finite number of modes), these different formula lead to different results and different convergence rates. In addition, even for one given formula of the excitation coefficient, there exist different formulations of the modal expansion of a physical quantity of interest, e.g., the scattering or the absorption cross-section. Therefore, a given physical problem can be represented by several modal expansions. It is important to test the convergence rate and the accuracy of these different modal expansion techniques for a finite number of modes.

We consider the calculation of the cross-sections (scattering, absorption, and extinction) of various plasmonic nanoresonators. We test different formulations of the quasinormal modes expansion as well as different closed-form expressions for the excitation coefficients. We provide a comparison of the convergence rate of each formulations of the modal expansion.

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Diatom frustules: A biomaterial with promising photonic properties

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Diatoms are an ecologically successful group of unicellular microalgae with a wide distribution into almost all aquatic ecosystems as well as a large share, both in the organic carbon world primary production and the released oxygen from photosynthesis process. Arguably, the most interesting structural feature of these microorganisms is their siliceous cell walls called "frustules". These frustules are produced through elegant biomineralization processes. Beside other interesting facts about diatoms, recent studies suggest that their frustules show amazing optical properties including the light focusing in centric diatoms [1], photonic crystal properties [2] and UV-induced photoluminescence. It has been suggested that these properties are correlated with photo-regulation processes in the living cells by e.g. keeping the photosynthetically active radiation near the chloroplasts, and protecting them from harmful wavelengths and high light intensities. Moreover, the frustules may play a role in low light environments by redistributing the light inside the cells. Due to these reasons, manipulation of the optical properties of diatom frustules might be also beneficial in optical application, and e.g. lead to more efficient solar energy harvesters, with diatom solar panels proposed for the production of both electricity as well as biofuels. The power of diatoms to work with light is both fascinating in itself, and can be a source for the development of new technologies [3]. In this poster, we illustrate the state-of-art for this recently arisen topic, and present our contribution to expand studies towards a clearer understanding of diatom frustule photonics, their roles in photobiology as well as in future optoelectronic applications.

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HighPerMeshes as a framework for numerical simulations

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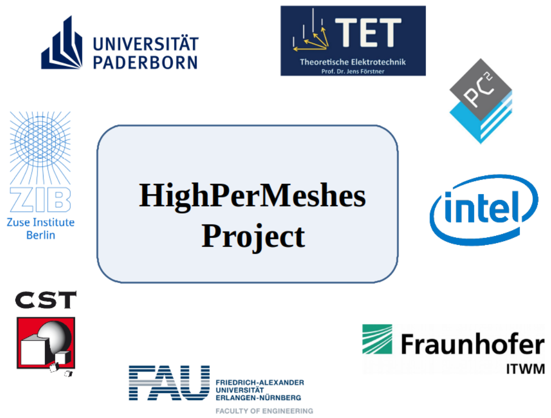
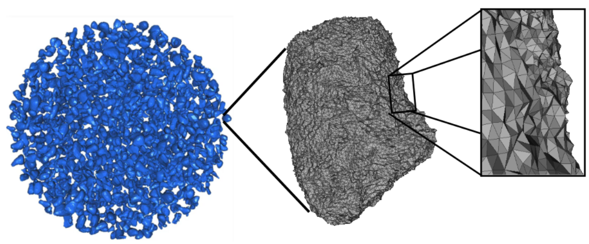
Due to the increasing necessity for large scale simulations and the growing availability of high performance computing we present a domain specific language (DSL) for application developers from science and industry areas to implement portable parallelized iterative algorithms productively on unstructured meshes.

Summary

HighPerMeshes is a BMBF (German Ministry of Education and Research) project targeting to develop a domain specific framework for large scale scientific simulations with non-regular discretization, which enables spatial flexibility with high accuracy in comparison to structured grids. The current example numerical methods include the discontinuous Galerkin method and the finite element method. The HighPerMeshes framework is developed in C++ and has the advantageous of portability on various computational architectures and super computing platforms (CPUs, GPUs and FPGAs) with efficient parallelization and scheduling. Thus there is no need to care about porting or parallelizing the code. This increases the productivity of the developers letting them concentrate on their own science and correctness of the results.



(a) HighPerMeshes project partners



(b) An example for a large scale Discontinuous Galerkin simulation (dust particles)

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Two-Color Soliton Compounds

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Numerical simulations of a nonlinear Schrödinger type equation shows a new kind of two-color ultrashort optical soliton bound states with moleculelike properties. These molecules have a strong binding energy, exhibit dipolelike radiation, and show dynamics of controlled fundamental soliton evaporation.

Solitons can be observed in a plethora of systems in nature and their interactions demonstrate analogies to different fields of physics. The most intriguing feature is their particle-like behavior, allowing a different view to the wave-particle dualism known from quantum mechanics. Soliton molecules that describe bound states of solitons are understood to be an extension of this analogy. Here we take the concept one decisive step further by demonstrating the existence of a previously unnoticed kind of soliton compound states in the nonlinear Schrödinger equation, exhibiting peculiar analogies to quantum mechanical binding energy, vibration, dissociation and dipole-like radiation [1]. The theoretical

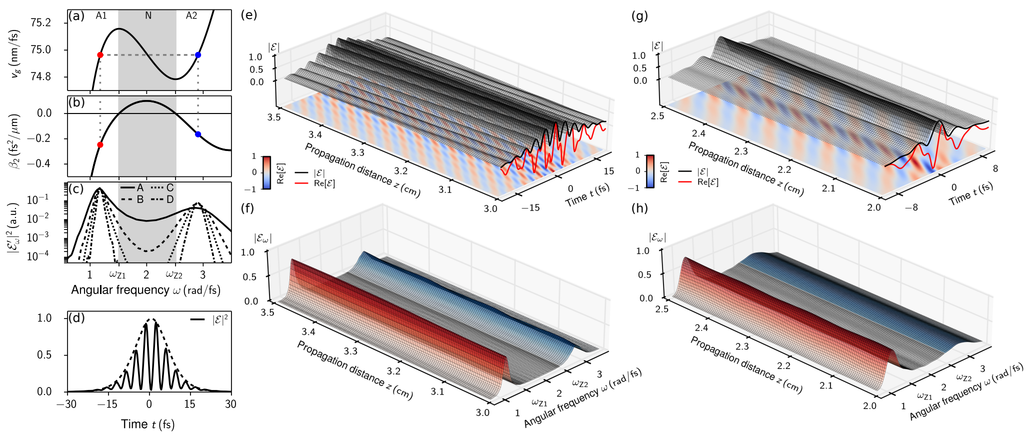

Fig. 1. Properties of the soliton molecules. (a) Group-velocity β_1 and (b) group-velocity dispersion profile β_2 with two regions of anomalous dispersion separated by a normal dispersion regime (gray shaded). (c) Spectrum of four different molecule states. (d) Temporal profile of selected soliton molecule. (e,f) Propagation of molecule state in time and spectral domain, respectively. (g,h) Same for ultrashort soliton molecule.

and numerical investigation of the propagation dynamics under perturbation, e.g., through subsequent collisions, or Raman scattering, reveals the robustness of these molecules. The dispersive character of the molecule after the separation of the constituents underlines that these states are not simply co-propagating solitons. The key point is to exploit the attractive potential between two incoherent ultrashort solitons. Besides fundamental interest these new molecules are promising for applications in ultrashort optical technologies due to their unique propagation dynamics, in communication systems as information can be decoded in the frequency domain, or for spectroscopy requiring coherent high-density spectra.

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Orbital Angular Momentum (OAM) Modes using Photonic Lanterns

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We present a mathematical model to design and analyze generation of vortex beams or orbital angular momentum (OAM) modes using photonic lanterns. The effect of various design parameters on the output OAM mode is discussed. A six-core photonic lantern has been used as an example for the study.

Vortex beams or orbital angular momentum (OAM) modes have gained considerable prominence in the field of optical fiber communication for mode division multiplexing [1]. Successful generation and application of OAM modes in free space optics [2] has led to a thrust in their study in fiber-based devices [1]. Photonic lanterns are novel photonic devices, which can be realized by adiabatically tapering a bunch of single mode fibers (SMFs) arranged within a low index capillary such that the tapered end is a few mode fiber (FMF) supporting as many modes as the number of SMFs. A six-core mode-selective photonic lantern [3] has been used as examples for this study. The device has a one to one correspondence between an input SMF core and an output FMF mode. Exciting two normalized inputs simultaneously can be mathematically expressed as

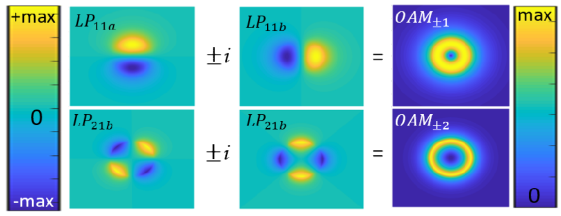

Fig. 1 Scheme for generation of OAM modes using pairs of LP modes.

$$|\psi\rangle_{out} = |s_a\rangle_{z_k} e^{-\int_0^{z_k} i\beta_a(z)dz+\varphi_a} + |s_b\rangle_{z_k} e^{-\int_0^{z_k} i\beta_b(z)dz+\varphi_b},$$

where $|s_{a,b}\rangle_{z_k}$ represent the mode field at the FMF end corresponding to the two inputs denoted by a and b, z_k is the device length, while $\varphi_{a,b}$ are the initial phases of the two inputs. The above expression is an outcome of the adiabatic theorem and uses the adiabatic propagation algorithm [4]. This propagation algorithm states that the coefficients of super modes excited at the input remain unaffected along the adiabatic taper. OAM mode generation as described in Fig.1 is very sensitive to the relative phase between the degenerate modes. Figure 1 shows the appropriate superposition of LP modes which are supported by optical fibers, FMF in our case for the generation of OAM modes. The propagation constants are computed at fixed intervals and interpolated to accurately obtain the corresponding acquired phase for each mode [4]. The input phases $\varphi_{a,b}$ are appropriately determined to obtain the required OAM mode. The phase and the amplitude corresponding to the OAM_1 and OAM_2 modes as obtained using the propagation algorithm [4] are shown in Fig.2. Detailed results shall be presented at the Workshop.

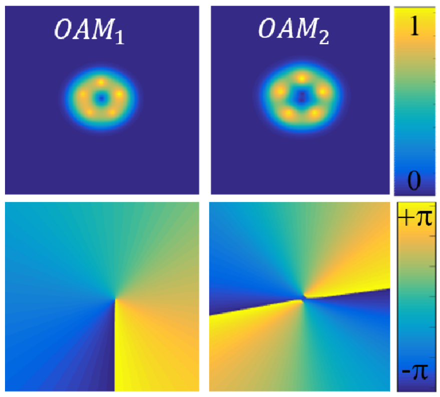

Fig. 2 Amplitude (top) and phase (below) of the generated OAM modes.

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Exploring the Absorption Mechanism in Numerical Boundary Conditions towards their Optimization

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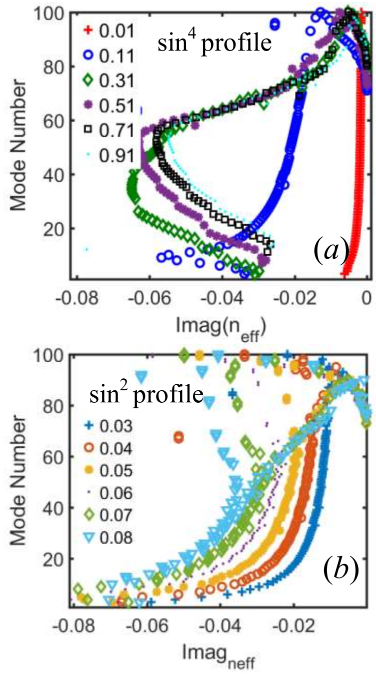
We explore the absorption mechanism in perfectly matched layer (PML) and absorbing boundary condition (ABC) in order to understand its effects of their performance. Our study based on modal analysis points towards possible conditions for optimal performance.

The absorbing boundary condition (ABC) [1] and the perfectly matched layer (PML) [2] are used to truncate the infinite transverse extent, ideally without affecting the propagation. This requires that the waves that are supposed to have left the computation window are absorbed in these layers without any reflection back into the computation window. In practice, we aim to minimize these reflections as these cannot be eliminated altogether. In both the PML and the ABC, the absorption effect inside the layer is made graded so that reflections at the interfaces and due the grading are minimized while the absorption is maximized. The profile of this variation (transverse coordinate in PML and the refractive index in ABC) plays a very important role in this optimization [3,4]. In this work we have examined the characteristics of the modes of the structure bound with the ABC/PML and have studied the efficiency of absorption of various profiles. We have used the collocation method for computing the modes [5]. We have considered a test case of a tilted Gaussian beam in a homogeneous media. It is found that the layer modes, *i.e.*, the modes that are confined to the absorbing layer have little or no role in the absorption of the Gaussian beam. It has been shown earlier [4] that some profile show better absorption than others. For example, the cubic and $\sin^4$ absorption profiles are better than the quartic and $\sin^2$ profiles in the ABC while quartic and $\sin^4$ profiles work better than square and $\sin^2$ profiles in the PML. The imaginary part of the effective indices of the modes show a particular trends for 'good' absorptions profiles while in the case of 'poor' profiles the trend is very different (see figures). Thus, by examining this behaviour one can choose a 'good' absorption profile without actually propagating a beam. We are now working on further classifying this behaviour.

Acknowledgment: *This work was supported through J.C. Bose Fellowship of the SERB, Govt. of India and 'Class of 66' Chair Professorship to Anurag Sharma.*



Imaginary part of the effective indices of various modes for (a) a 'good' and (b) a 'poor' absorption profiles in the ABC. Various curves correspond to different strength of the absorption as shown. Layer width is 24% of the total window.

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Finite Element Simulation and Optimization of Inverted Plasmonic Lenses

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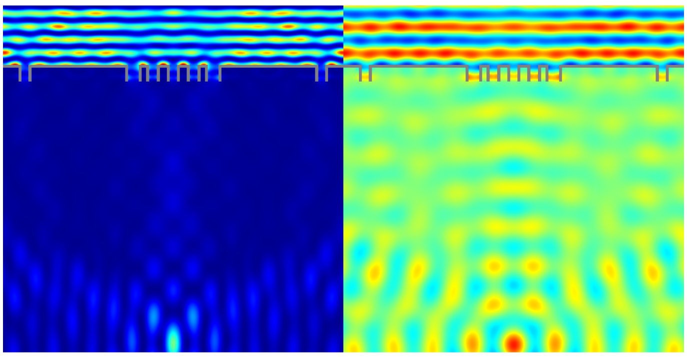
We present a new design scheme for plasmonic nanoslit lenses, the inverted plasmonic lens, which accommodates lithographic fabrication processes. We used the finite element method to simulate lenses with varying parameters and design a set of lenses for the application at visible and near-infrared wavelengths.

Concerning the characterization of nanostructures, imaging Mueller matrix ellipsometry has shown potential to reveal subwavelength form information by the off-diagonal elements of the Mueller matrix [1]. For a sensitivity enhancement of these features, we study the application of plasmonic lenses in ellipsometry setups. Conventional plasmonic nanoslit lenses consist of purely metallic slabs with slit arrays working as phase delaying waveguides for surface plasmon polaritons (SPPs) [2]. The aspect ratios of these slits are required to be very high, resulting in a demand for slits with only a few tens of nanometres in width through metallic layers with a thickness of up to 2 μm, which is challenging for the fabrication process.

In this contribution, we discuss a new design scheme, called the inverted plasmonic lens. It consists of dielectric ridges which are covered with a metallic layer to maintain SPP propagation. This design allows for an easier fabrication by means of electron beam lithography for the dielectric ridges combined with atomic layer deposition to produce the metallic coating. We used the finite element method tool JCMwave to simulate inverted plasmonic lenses with different parameters. To improve the geometrical parameters with regard to the optical performance of the lens compared to the conventional design as well as to preliminary results, we combined the numerical simulations with optimization algorithms. By this, we designed a set of lenses that can be applied in the visible and near-infrared wavelength regime with focal lengths between 5 μm and 1 mm. The inverted plasmonic lenses show focal spots with intensities comparable to the conventional design and spot sizes of less than half of the incident wavelength.



Inverted plasmonic lens (grey structure indicating the metallic coating), illuminated by a plane wave from above. Intensity (left) and amplitude distribution (right). In the desired distance the lens produces a focal spot.

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Analysis of ellipsometric layer thickness measurements employing a new merit function for depolarizing Mueller matrices

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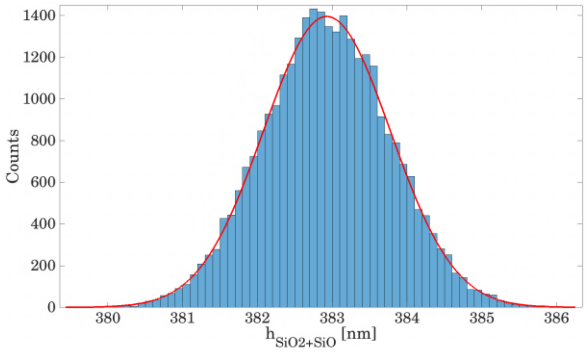
We developed a new optimization method for the analysis of depolarization containing Mueller ellipsometric measurements. Applied on measurements of layer thickness standards we demonstrate a significant conformity of our ellipsometric results to those traced by traceable X-ray reflectometry (XRR) at PTB.

Spectroscopic ellipsometry is widely used to measure dimensional or optical parameters of surface layers or structures. This is done by solving an inverse problem via an optimization process, where simulated and measured quantities are compared. In general, Maxwell's equations must be solved numerically for simulation of the light-surface interaction in the measurement process. For unstructured layers it is sufficient to apply Fresnel-equations.

Our goal is to establish traceable and reliable Mueller matrix ellipsometric (MME) measurements. Up to now a mathematically well-founded treatment of stochastic influencing parameters such as depolarization or measurement noise is missing, impeding complete uncertainty considerations.

Therefore, for the first time we addressed these issues: we developed a new optimization method for depolarizing Mueller matrices ([1]). Depolarization is addressed here as a weight ([2]) by applying Cloude's covariance matrix ([3]). This also enables to use the maximum likelihood method and Bayesian statistics via the Markov Chain Monte Carlo technique. Moreover, an extension has been implemented which allows to include measurement noise into this merit function. Typically, another significant uncertainty contribution results from the uncertainty of the selection of the right surface models. We solved this issue by using the Bayesian information criterion.



Probability distribution of combined SiO_2+SiO layer thickness

We applied the new method on measured data of SiO_2 layer thickness standards with nominal heights between 6 nm and 1000 nm, which have been measured by a SENTECH Mueller ellipsometer. The necessary and successful use of Bayesian statistics to determine the underling height distributions will be presented. Finally, the mean values and extended uncertainties from our measurements will be compared to those traced to XRR at PTB. The excellent matching significance is shown by the obtained normalized error values E_n.

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Multipolar decomposition of quasi-normal modes: a new design tool for nano-optics

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We develop a rigorous multipolar theory of QNMs to design a nanoparticle exhibiting a completely original optical behavior that is broad both spectrally and angularly. Our design strategy is illustrated by designing a subwavelength optical resonator exhibiting a Janus resonance that provides side-dependent coupling to waveguides.

Abstract

Interference between multipole moments of photonic or plasmonic nanoresonators or meta-atoms - is known to lead to many exotic phenomena, like zero forward or backward scattering, supper scattering, Fano resonances, and non-radiating anapole responses. A standard approach to analyze the multipolar response of a nanoresonator consists in decomposing the field scattered by it under planewave excitation in terms of radiating multipoles. Because this analysis is generally made at specific frequencies and incident angles, the targeted optical response is usually obtained for narrow spectral and angular ranges, thereby seriously limiting the applicability of the designed nanoresonator for practical applications. As we now know, however, the optical response of a nanoresonator is fundamentally driven by its natural resonances the so-called Quasi-Normal Modes (QNMs) which are source-free solutions to Maxwells equations [1]. Recent work has suggested that individual resonances, i.e. QNMs, could exhibit a given multipolar content [2], suggesting the possibility to design nanoresonators with an optical response that is insensitive to the external source.

Here, we develop a rigorous multipolar theory of QNMs and exploit it to design a nanoparticle exhibiting a completely original optical behavior that is broad both spectrally and angularly [3]. A rigorous numerical approach for the multipolar decomposition of resonances at complex frequencies is presented, along with an analytical model conveying a direct physical insight into the multipole moments induced in the resonator. Our design strategy is illustrated by designing a subwavelength optical resonator exhibiting a Janus resonance [4] that provides side-dependent coupling to waveguides over the full linewidth of the resonance and on a wide angular range for linearly-polarized incident planewaves. The method applies to all kinds of waves and may open new perspectives for subwavelength-scale manipulation of scattering and emission.

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Analysis of Open Elliptical Nanophotonic Structures with the Modal Method

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In this contribution, open boundary elliptical nanophotonic structures are modeled and simulated via a full-wave vectorial modal method. Analytical basis modes based on the splitting of transverse magnetic and transverse electric fields are constructed. The special basis modes used in the implementation lead to analytical coupling integrals, and therefore fast and efficient simulations.

Introduction

Transforming foundational knowledge into real applications requires high-efficiency devices. This is not different for quantum and laser photonics [1]. To design efficient photonic structures, one needs to have a powerful, efficient simulation tools at hand. The modal method provides not only rigorous solutions to electromagnetic problems but also provides an understanding of the phenomenon via direct access to physical quantities such as propagation constants, eigenmodes, and modal reflection coefficients. That access eases the calculation of spontaneous emission rates and of β factors of lasers and single-photon sources significantly.

Elliptical structures are known to allow polarization control and true-monomode operation capabilities [2]. Their simulation with traditional full-wave solvers such as the Finite Element Method or the Finite Difference Time Domain Method are computationally expensive. Those methods employ absorbing boundary layers which have to be tuned to model the open boundary environment. However, with the modal method exploiting the symmetry of the structure and modeling intrinsically the correct boundary conditions, it is possible to implement an efficient solver without such artificial layers.

Method

We expand transverse fields in terms of known basis modes and unknown modal coefficients. We employ a splitting in the basis modes based on transverse magnetic and transverse electric fields, unlike the splitting based on coordinate variables usually applied in the literature [3]. We obtain the basis modes from analytical solutions of the empty geometry. That leads to analytical coupling integrals which can be evaluated easily. The open boundary environment is taken into account by discretizing non-uniformly the infinite k-space domain [4]. That further increases the stability and efficiency of the solver.

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Ultra-short Optical Pulse Dynamics in Bidirectional Ring Fibre Cavity

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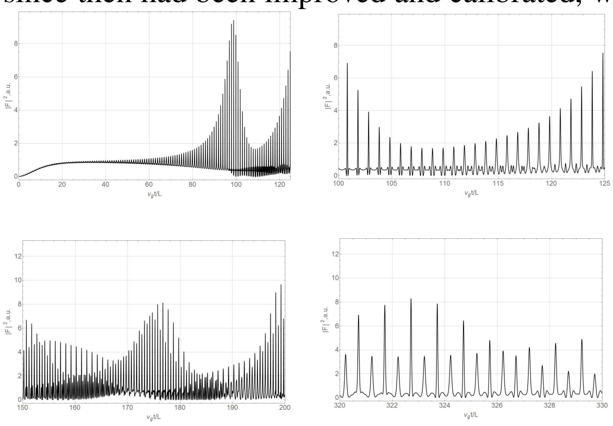
A new applied realization of the “Cabaret” numerical method is offered, investigating long-time spatio-temporal dynamics of the electromagnetic field in a nonlinear ring cavity with dispersion during the hundreds of round trips. Two waves run in the opposite directions and influence each other. Formation of temporal cavity solitons, regular and irregular pulse trains is demonstrated and discussed.

Model Description

We investigate the dynamics of a cavity that includes coupler, through which both continuous wave pumping and output occur, and a classical mirror somewhere along the cavity length. This system is mainly used as a really simple approach for optical comb generation, or supercontinuum generation. In this case there are two waves in the cavity propagating in the opposite directions. There is dispersion present in the cavity, as well as the Rayleigh scattering and nonreciprocal phase shift. We have presented our model that uses upwind methods back in 2016 [1], and the model since then had been improved and calibrated, with the results published over the passed years [2, 3].



Examples of the modelling results. The top row displays the dynamics of the pulse propagation as a whole, unidirectional case with the dispersion. The bottom row displays the close up cuts of the regimes where the fibre has received nonreciprocal phase shift because of the slight rotation introduced, and there is a highly reflective intra-cavity mirror installed. Introducing of the Rayleigh scattering significantly changes the dynamics.

Conclusions

Summarizing, we can state that we’ve managed to create a stable and quite accurate numerical model that allows us to account for a wide range of the linear and nonlinear effects as needed in any given problem. Our goal is to investigate the obtained results and further improve our modelling methods.

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Global optimization of a free-form waveguide coupler

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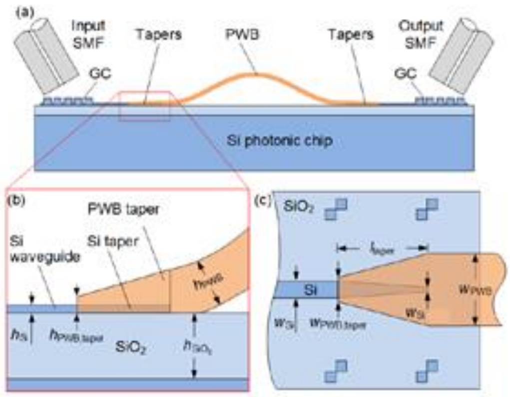
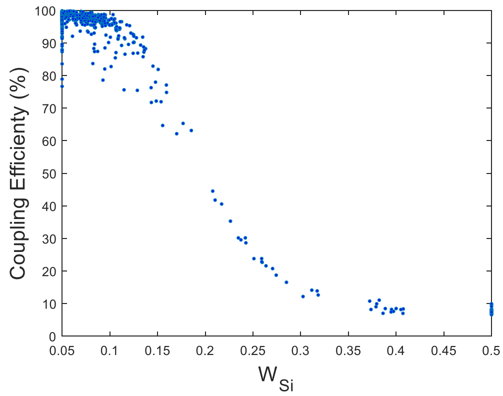
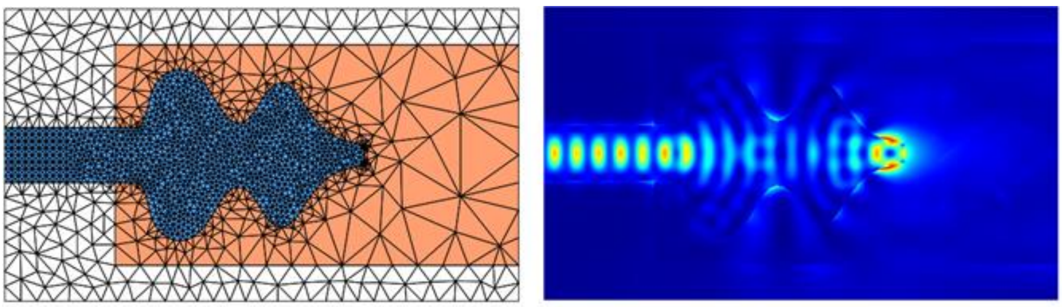
We optimize a waveguide coupler for a photonic integrated inter-chip communication system[1]. In order to reduce the surface area of the coupler, we analyze the performance of compact free-form non adiabatic designs. The optimization is done combining Bayesian optimization[2] and the use of shape derivatives. The coupler is optimized for a central wavelength of λ = 1550 nm and a bandwidth of 300 nm.



Schematic and field profile of the adiabatic waveguide coupler.



Coupling efficiency of the adiabatic coupler.



Mesh grid and field profile of a 2D free-form model.

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Wave Processes in Tunable Layered, Nonlinear, Active and Mesoscale Hyperbolic and Dielectric-Graphene Metamaterials

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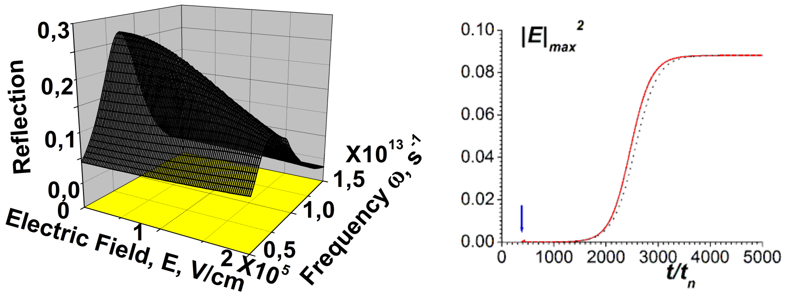
The capabilities of (i) effective resonant control of nonlinear conductivity and modulation of the electromagnetic beam in multilayer dielectric-graphene-dielectric ... metamaterial (DGMM) placed in a magnetic field in the THz range and (ii) the development of a synergetic process with the absorption by an infrared (IR) pulse of the other pulses entering into the layer of active nonlinear hyperbolic metamaterial (ANHMM) with linear amplification and saturation, are demonstrated, for the first time.

Using two methods, hydrodynamic and kinetic, the possibility of effective nonlinear resonance modulation of the conductivity of graphene and electromagnetic beams (Fig. 1a) in DGMM is shown. The passage of electromagnetic IR pulses which incident obliquely onto the ANHMM layer is modeled on the basis of a system of coupled Maxwell-Bloch equations. In the metamaterial approximation, the modified Ginzburg-Landau equation with complex coefficients including the group velocity and a term with a mixed spatial derivative is derived, for the first time. In the presence of pure linear amplification, it turns out to be necessary to consider the mesoscale regime of work of ANHMM [1]. In this case, instead of the (metamaterial) approximation of a continuous medium with averaging over nanolayers containing in an ANHMM elementary cell (which includes an additional dielectric layer with an active medium), the wave equations for each layer are solved with the corresponding matching of fields between neighboring layers. Both methods demonstrate (i) the possibility of hot spot formation under a condition of an attenuation compensation [1] and (ii) the aforementioned synergetic process in ANHMM with saturation of the pulse amplitude (Fig. 1b) in the presence of resonant nonlinear dissipation in the active layers.



a *b*

Figure 1. a-dependence of the reflection of THz electromagnetic beam incident normally on DGMM with a single resonant graphene layer placed in a normal magnetic field, on the amplitude of electric field E and carrier frequency ω of incident beam; b- the amplification with saturation of two small input pulses of different amplitudes incident on a layer of ANHMM; the incidence angle of a pulse on ANHMM layer is $\theta_i = 30^o$; the time of the incidence of the input pulse is marked by arrow.

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New Physical Phenomena: Switching of Focusing and Chaotic Field Behavior in Strongly Nonlinear Active Hyperbolic Field Concentrator

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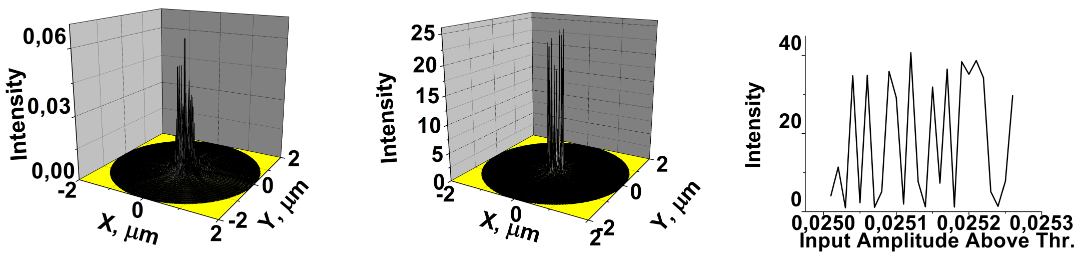
A new physical phenomenon has been discovered: a threshold jump in the position of the focusing point with the formation of a hot spot (s) and the above-threshold quasi-chaotic behavior of a field in a hyperbolic nonlinear cylindrical field concentrator to which infrared (IR) beam(s) fall(s) from outside. The scenarios of the transition of the system to such a strongly nonlinear state are investigated.

The 2D model of the new type of field concentrator [1] includes a cylindrically-symmetric region of an active hyperbolic metamaterial of finite radius with an axis directed along the axis z using a cylindrical coordinate system (z,ρ,ϕ), while $\partial/\partial z=0$. A beam with IR carrier electromagnetic mode with field components (H_z, E_ρ, E_ϕ) is considered. The external and inner regions of active hyperbolic field concentrator (AHFC) are linear and non-linear (with focusing non-linearity), respectively. The distribution of intensity in the inner region of AHFC in the subthreshold and suprathreshold modes (with jump of intensity) are shown in Figs. 1 a and b, respectively. We revealed the nonlinear focused structures of three main types: (i) symmetrical ones with maxima distributed along the circle around the center of AHFC with a radius of order of carrier wavelength in free space; (ii) ones with maxima of intensity distributed around the (circle) boundary between the external linear and internal nonlinear regions of AHFC; (iii) hot point- like structures, shifted respectively to the center of AHFC. We have proposed a set of different methods of controlling the jump of focusing point and switching maximum intensity level, such as (i) changing level of the input signal; (ii) using extra weak controlling beam with controllable intensity; (iii) changing linear gain/compensating linear losses in AHFC; (iv) variation of the nonlinear losses in the AHFC etc. In all these cases we obtained qualitatively the same effect of the jump of focus point and switching (jumping) the maximal intensity in the nonlinear region of AHFC. Chaotic-like behavior of the intensity in the region of focusing in the suprathreshold regime is found and illustrated in Fig. 1c.



a b c

Figure 1. (a) u (b)- the intensity distribution of the concentrated field of beams incident from the outside on the AHFC in the internal nonlinear region at subthreshold and suprathreshold (with a jump in intensity) values of amplitudes of the incident beams in the focusing region, respectively;coordinates x, y are lying in the plane (ρ,ϕ); *(c)-chaotic-like dependency of the field intensity in the region of focusing in the suprathreshold regime, on input beam amplitude.*

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